Energy Transition
RESEARCH & INNOVATION

SÃO PAULO, BRAZIL | NOVEMBER 7-9, 2023

Energy Transition Research & Innovation Conference

ETRI 2023

BOOK OF ABSTRACTS

Research Centre for
Greenhouse Gas Innovation

USP

FAPESP

ETRI 2023 was sponsored by

Energy Transition Research & Innovation Conference

ETRI 2023

São Paulo, November 7-9, 2023

BOOK OF ABSTRACTS

ETRI Organization:
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Julio Romano Meneghini – Conference Co-Chair
Suani T. Coelho – Scientific Committee Chair
Alberto José Fossa – Scientific Committee Co-Chair

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SUMMARY

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WELCOME WORDS

Welcome to the Book of Abstracts of the 6th Energy Transition Research & Innovation Conference (ETRI 2023)!

The Research Centre for Greenhouse Gas Innovation (RCGI) at the University of São Paulo (USP) extends a warm welcome to all readers. ETRI 2023, partially sponsored by Shell, was held from the 7th to the 9th of November 2023 at USP's vibrant Campus Butantã. It showcased groundbreaking advancements and fostered an environment of collaboration and innovation.

This year marked a significant milestone as ETRI opened its doors to academic institutions beyond USP, as well as industry and government representatives. The enthusiastic response was overwhelming, with 542 attendees—an impressive 116% increase from last year's conference. Among the participants were 384 RCGI researchers, 58 external researchers, 25 government officials, 12 industry leaders, and 22 journalists, all contributing to a dynamic and diverse gathering.

The event was structured to maximise engagement and knowledge exchange, featuring an opening ceremony, four keynote speakers, eight panels, twenty short oral sessions, and a closing ceremony where we honoured excellence with the ETRI Excellence Awards. With 52 speakers and 21 esteemed professors on the Scientific Committee covering nine thematic tracks, the conference buzzed with insightful discussions and presentations, all organised into four parallel sessions daily.

We were privileged to host distinguished speakers like Ambassador André Correa do Lago, Professor Dr Vahan Agopyan, Professor Dr Carlos Nobre, Plinio Nastari – founder of DATAGRO, Olivier Wambersie – General Manager of Technology and Innovation at Shell Brasil, and Elbia Gannoun CEO from Abeeolica, among other notable experts. Their contributions enriched the conference, providing diverse perspectives and expertise on the pressing issue of energy transition.

This year's ETRI saw a record number of 226 abstracts, a 35% increase from 2022, with 22% coming from external participants—a testament to the growing interest and collaborative spirit in the field of energy transition. The conference also enjoyed substantial media coverage with more than 60 organic publications and significant engagement on RCGI's social media platforms, underscoring the broad interest and commitment to energy innovation from all sectors of society.

We present the culmination of these efforts in the Book of Abstracts of ETRI 2023. It encapsulates the rich array of research and ideas presented during the conference's twenty short oral sessions, highlighting the work of 226 dedicated researchers. We are thrilled to share this wealth of knowledge with you and look forward to continuing this journey of discovery and innovation together.

Thank you for being a part of this remarkable event. We eagerly anticipate welcoming you to the next ETRI in 2024!

With warm regards,

Karen Louise Mascarenhas
Conference Chair

Julio Romano Meneghini
Conference Co-chair

Suani T. Coelho
Scientific Committee Chair

Alberto Fossa
Scientific Committee Co-chair

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THEMATIC TRACK

1 - Natural Based Solution (NBS)

This thematic track involves the restoratin of native vegetation, expansion of integrated agricultural systems and the restoration of pasture areas. In addition, the track also considers techniques to restore vegetation, re-establishing native species. In this way, the soil will accumulate a high biodiversity of plant substrates that should stimulate its microbial biomass, resulting in potential carbon fixation in the soil.

2 - Carbon Capture Utilization and Storage (CCUS)

This thematic track focuses to create value from CO2 emissions through the design of integrated processes for CO2 capture and conversion. In this concept, CO2 is considered a valuable chemical building block for fuels and materials. This track also includes technologies used in CO2 storage in geological structures and other types.

3 - Bioenergy with Carbon Capture Use and Storage (BECCUS)

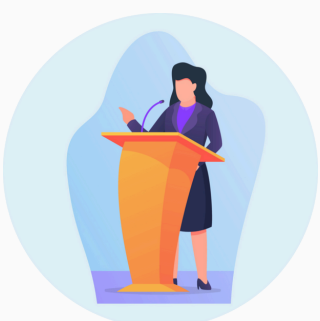
This thematic track involves technologies or a set of technologies that associate biomass energy with carbon capture use and storage, a process always carried out on a large scale. With this it is possible to sequestre carbon from the atmophere. Works that present the technologies and their contribution to building a positive public perception of BECCUS influencing the design of public sustainability politicies for the Brazilian energy systems are included.

4 - Greenhouse Gas (GHG) Technologies

The Greenhouse Gas (GHG) Programme is dedicated to study technologies related to Measurement and quantification of GHG emissions; Mitigation of GHG emissions, such as, pneumatic machines and devices in general, Chemical looping combustion and Oxy-fuel combustion; Adsorption systems for CO2 capturing from flue gases; Deep eutectic solvents for CO2 capture from flue gases; and Membranes for CO2 capture from flue gases.

5 - Standardization, Regulation, Social Perception & Acceptance

This thematic track is related to the development of documents for climate change, sustainable and decarbonization fields, such as requirements standards, specifications and guides, which can be used to consistently ensure that material, products, processes and sevices are suitable for its purposes. This track also supports policies to provide the energy transition and societal engagement, achieved by the understanding of the social perception and acceptance of all stakeholders as well as the lay public, establishing an open dialogue with society. Works and studies in these areas are key to support technology transition and implementation.



6 - Environmental, Social & Gender

This track intends to receive papers to discuss environmental impact and social aspects of Energy Transition including but not limited to gender and justice issues, energy access and safety, poverty aliviation, women participation, development of economic activities among others.

7 - Energy Transition Economics & Carbon Credits

Economic papers of energy transition, including economic feasibility of renewables and non renewables, as well as how carbon credits can contribute to Energy Transition feasibility. What are the challenges and benefits for policies related to carbon credits, as well as SWOT analysis.

8 - Energy Management & Saving

This track involves energy management as an opportunity to enable organizations across all sectors to realize on-going energy consumiption reducion and related GHG emissions reduction. This thack includes activities and technologies for establishment, implementation and maintanance of energy management systems, monitoring and measuring energy performance for continual improvment; identifying, quantifying, verifying, validating and reporting energy performance improvements; energy security; energy savings calculations; terminology, competencey and conformity assessment in this field.

9 - Power & Storage

This thematic track seeks to present innovative and sustainable solutions focused on the decarbonization of electrical power systems. It includes but not limited to aspects such as eco-efficient materials, increased availability and efficiency of electricity production, optimization of distributed energy resources and integration with agriculture, digitalization of eletricity.

Energy Transition
RESEARCH & INNOVATION

GENERAL PROGRAMME

TUESDAY, 7 NOVEMBER 2023

8:30 REGISTRATION & WELCOME COFFEE.

9:30 OPENING CEREMONY.
Prof. Dr. Vahan Agopyan - State Secretariat of Science, Tecnology & Innovation.
Prof. Dr. Susana Inés Córdoba de Torresi - Provost for Research at USP.
Mr. Daniel Maia Vieira - Technical Director National Agency for Petroleum, Natural Gas and Biofuels (ANP).
Dr. Carlos Américo Pacheco - Chief Executive Officer Technical and Administrative, FAPESP.
Dr. Olivier Wambersie - General Manager R&D and Innovation, Shell.
Prof. Dr. Julio Meneghini - RCGI Scientific Director, University of São Paulo.
Prof. Dr. Karen Louise Mascarenhas - ETRI 2023 Chair Conference.

10:10 KEYNOTE TALK.
Keynote 1: Brazil's Role in the Global Energy Transition.
Chair: MsC. Camila Farias - Industry Vice Director at RCGI & Technology Project Lead Shell Brasil.
Dr. Olivier Wambersie - General Manager R&D and Innovation, Shell.

11:00 LAUNCH: OTIC - Offshore Technology Innovation Centre (OTIC).
Prof. Dr. Kazuo Nishimura - OTIC Executive & Scientific Director.

11:10 Panel 1: Energy Transition to Combat Climate Change: What Policies Are Necessary?
Chair: Prof. Dr. Patricia Iglesias - Head of Environment - University of São Paulo.
Prof. Dr. Vahan Agopyan - State Secretariat of Science, Technology and Innovation.
Dr. Marisa Maia de Barros - Undersecretary of Energy and Mining at the Secretariat of Environment, Infrastructure, and Logistics of the Government of the State of São Paulo.
Dr. Angela Oliveira da Costa - Head of Oil Products and Biofuels Studies Department, Brazilian Energy Research Office.
Dr. Plinio Nastari - Founder and President at DATAGRO Consulting.
Dr. Fabio Feldman - Fabio Feldman Consultores.

12:30 LUNCH BREAK.

14:00 KEYNOTE 2: Brazilian NDCs: the way forward.
Chair: Prof. Dr. Suani T. Coelho - RCGI – IEE – USP / GBio.
Ambassador André Correa do Lago - Secretary of Climate, Energy and Environment of the Ministry of Foreign Affairs.

14:50 KEYNOTE 3: How to fight deforestation in the Amazon Forest?
Chair: Prof. Dr. Paulo Artaxo - Physics Institute, USP.
Prof. Dr. Carlos Nobre – Institute of Advanced Studies, USP.

15:40 COFFEE BREAK.

16:00 PANEL 2: How can Technology & Research & Innovation support Energy Transition?
Chair: Prof. Dr. Julio Meneghini - Executive & Scientific Director RCGI.
Prof. Dr. Anthony Kucernak - Professor of Physical Chemistry in the Department of Chemistry, Imperial College London.
Prof. Dr. Andre Faaij - Director of Science TNO Energy & Materials Transition & Professor Energy System Analysis at Copernicus Institute of Sustainable Development, Utrecht University.
Prof. Dr. Chinnakinda S. Gopinath - Outstanding Scientist - Institute National Chemical Laboratory, Pune, India.
Prof. Dr. Ana Flavia Nogueira - Full Professor at the Institute of Chemistry at the University of Campinas (UNICAMP) and Director of the Center for Innovation in New Energies.
Prof. Dr. Paulo Artaxo - Physics Institute – USP.
MsC. Alexandre Breda - Low-Carbon Technology Manager Shell Brazil.

17:20 SHORT-ORAL SESSION A.

18:30 CLOSING OF THE DAY.

WEDNESDAY, 8 NOVEMBER 2023

8:30 WELCOME.

8:50 OPENING SESSION.

9:00 PANEL 3: Pathways to achieve Net Zero.
Chair: Prof. Dr. Carlos Frederico de Oliveira Graeff - General Coordinator of Strategic Programs and Infrastructure FAPESP.
Prof. Dr. Carlos Eduardo Cerri - RCGI Director of the Nature Based Solutions (NBS) Programme.
Prof. Dr. Pedro Vidinha - Assistant Professor USP - Carbon Capture and Utilization (CCU).

Prof. Dr. Marcos Buckeridge - RCGI Director of the Bioenergy with Carbon Capture and Storage (BECCS) Programme.
Prof. Dr. Emilio Nelli Silva - RCGI, Deputy Scientific Director & Director of Greenhouses Gases (GHG) Programme.
Prof. Dr. Edmilson Moutinho dos Santos - RCGI Director of the Advocacy Programme.
Prof. Dr. Maurício Salles – RCGI Director of Power Systems Innovation Hub, InnovaPower Programme.

10:10 SHORT-ORAL SESSION B.

11:10 COFFEE-BREAK.

11:30 SHORT-ORAL SESSION C.

12:30 LUNCH BREAK.

14:00 PANEL 4: Carbon Credits and Economics as key enablers for the energy transition.
Chair: Prof. Dr. Virginia Parente - Professor at the Institute of Energy and Environment, USP.
Prof. Dr. Ariaster Baumgrat Chimeli - Professor at FEA, USP.
Prof. Dr. Gesner Oliveira - Professor at Fundação Getúlio Vargas (FGV), Coordinator of the Center for Infrastructure and Environmental Solutions Studies.
Dr. Viviane Romeiro - Director of Climate, Energy and Sustainable Finance - Conselho Empresarial Brasileiro para o Desenvolvimento Sustentável - CEBDS.
Dr. Agnes Maria de Aragão da Costa - Director of the Brazilian Electricity Regulatory Agency (ANEEL).
Prof. Dr. José Roberto Moreira - Senior Professor at the Institute of Energy and Environment of the University of São Paulo.

15:20 SHORT-ORAL SESSION D.

16:20 COFFEE BREAK.

16:40 PANEL 5: "What is the role of the start-ups in the Energy Transition?"
Chair: Dr. Isabela Morbach - CCS Brasil.
Dr. Alexsandro Kirch - Multiscale.
Dr. Dagoberto Silva - Moftech.
Dr. Deise Nogueira - Quanticum.
Dr. Maitê Lippel Gothe - Carbonic.
Prof. Dr. Marcelo Rodrigues - Krilltech.

18:00 CLOSING OF THE DAY.

THURSDAY, 9 NOVEMBER 2023

8:30 WELCOME.

8:50 OPENING.

9:00 PANEL 6: The Role of Women in Energy Transition aiming to achieve the Sustainable Development Goals.
Chair: Prof. Dr. Karen L. Mascarenhas - Conference Chair, RCGI USP.
MsC. Camila Farias - Industry Vice Director at RCGI & Technology Project Lead Shell Brasil.
Dr. Elbia Gannoun - CEO of Brazilian Association of Wind Energy and New Technologies (ABEEólica).
Prof. Dr. Suani T. Coelho - RCGI – IEE – USP / GBio.
Prof. Dr. Telma Teixeira Franco - Professor of Bioengineering at University of Campinas (UNICAMP).
Prof. Dr. Virginia Parente - Professor at the Institute of Energy and Environment - USP.

10:10 SHORT-ORAL SESSION E.

11:10 COFFEE-BREAK.

11:30 PANEL 7: **The evolution of the SDGs in Brazil.**
Chair: Prof Dr Arlindo Philippi - Rector's chief of staff USP.
Mr. Sergio Murilo - Chief of staff at the federal senate
Prof. Dr. Patricia Iglecias - Head of Environment - University of São Paulo.
Prof. Dr. Suani T. Coelho - RCGI – IEE – USP / GBio.
Dr. Tamar Roitman - Executive manager at Associação Brasileira de Biogás (ABiogás).

12:30 LUNCH BREAK.

14:00 SHORT-ORAL SESSION F.

15:00 KEYNOTE 4: From bench to business – innovations in electrochemical technology for the low carbon energy transition.
Chair: Prof. Dr. Thiago Lopes - RCGI, USP.
Prof. Dr. Nigel Brandon OBE FREng FRS - Dean of the Faculty of Engineering at Imperial College London.

16:00 COFFEE-BREAK.

16:20 PANEL 8: Highlights & Challenges of the Brazilian Energy Transition.
Chair: Dr. Alberto Fossa - Co-Chair of the Scientific Committee.
Dr. Pedro Vidinha - Assistant Professor USP - Carbon Capture and Utilization (CCU).
Prof. Dr. Lucy Sant'Anna - CCUS Thematic Track Leader.
Prof. Dr. Danielle Denny - NBS Thematic Track Leader.
Prof. Dr. Marcos Buckeridge - BECCUS Thematic Track Leader.
Prof. Dr. Renato Picelli - GHG Thematic Track Leader.
Prof. Dr. Karen L. Mascarenhas - Conference Chair, RCGI USP.
Prof. Dr. Suani T. Coelho - EnvGS Thematic Track Leader.
Prof. Dr. Virginia Parente - ETE Thematic Track Leader.
Prof. Dr. Mauricio Salles - PS Thematic Track Leader.

17:20 CEREMONY - ETRI 2023 Excellence Award.

18:00 CLOSING OF THE DAY.

Energy Transition
RESEARCH & INNOVATION

SHORT ORAL SESSION PROGRAMME

TUESDAY, 7 NOVEMBER 2023

0711 - NBS1 (TV1)

NBS Carlos Cerri - Mauricio Cherubin

Alisson Luiz Rocha Balbino	Exploring Metal Organic Frameworks Synthesis: A Comparative Analysis of Hydrothermal and
Ana Paula Cervi Ferez	Novel field-based models to monitor carbon stocks of forest under restoration in
Antonio Yan Viana Lima	Grazing exclusion: a nature-based solution to increase microbial activity in Brazilian desertified drylands
Beatriz da Silva Vanolli	Carbon stock dynamics in short-term integrated agricultural systems on sandy soils
Bruna Emanuele Schiebelbein	Status of soil health in agricultural soils in Brazil using the Soil Management Assessment Framework
Bruna Gonçalves de Oliveira Carvalho	Distinguishing microbial pathways responsible for n2o emissions in soils under
Catharina Weber Neiva Masulino	Nature-Based Solutions (NBS) and the Integration of Local Communities: A Sustainable Path for Socio-
Crislany Canuto dos Santos	Integration crop-livestock-forest systems influence soil c stock in the semi-arid of Ceara
Daniela Higgin Amaral	Projections of sustainable forest biomass demand as energy source in Mato Grosso
Letícia Beatriz Ueda Melo	From Vinasse Pollution to Green Resource: Microalgae-Assisted Biomolecule Accumulation and Toxic Compound Removal

SHORT ORAL SESSION PROGRAMME

TUESDAY, 7 NOVEMBER 2023

0711 - CCUS2 (TV2)

CCUS Colombo Tassinari – Renato Gonçalves

Fagner Rodrigues Todão	The Role of N-Doped Carbon Structures in the Thermocatalytic CO2 Hydrogenation over Co/SiO2 Catalysts
Jean Castro da Cruz	Development of catalytic pathways for CO2 transformation into chemicals and materials
Giliandro Farias	A combined DFT and machine learning study to understand catalyst and solvent effects on the conversion of CO2 into ethanol
Dyovani Bruno Lima dos Santos	Exploring the Impact of Various Supports on K-Promoted Molybdenum-Based Catalysts for CO2 Hydrogenation Reaction
Adolfo Lopes de Figueredo	Tuning catalytic hydrogenation of fumaric acid with supercritical CO2 for GBL and THF production
Jorge Andrés Mora Vargas	Synthesis of New Polyurethanes from Biomass-derived Monomers
Giovanni Rodrigues Morselli	Interactions between CO2 and superbase in ionic liquids probed by vibrational spectroscopy
Gabriel Silveira dos Santos	Development of new deep eutectic solvents from low molecular mass hyperbranched polyglycerolsassociated with superbase for carbon dioxide absorption.

SHORT ORAL SESSION PROGRAMME

TUESDAY, 7 NOVEMBER 2023

0711 - PS8 (TV3)

CCUS Colombo Tassinari - Renato Gonçalves

Kalisye Rodrigues Gilini	Optimization Methodology for Local Control for Efficient Integration of Distributed Energy Resources – PS156
Lucas Santos Figueiredo	Development of a Type III generator model for electrical resonance studies in wind farms – PS150
Luís Fernando Nogueira de Sá	Optimizing PEM Fuel Cell Performance with a Pseudo-3D Approach – PS151
Luiza Buscariolli	Methodologies for Resonance Analysis in Power Systems with Wind Generation – PS152
Maria Paula de Souza Rodrigues	Utilizing MnO2 Nanowires as Cathodes in Sodium-Ion Batteries Employing Water-in-Salt Electrolytes – PS153
Mário Oleskovicz	Fault location of onshore wind farm collector network based on artificial intelligence and drone supervision ("faultAIfinder") – PS154
Marilin Mariano dos Santos	Strategic route for CO2 transportation in the state of Rio de Janeiro – PS155
Marilin Mariano dos Santos	Long-term offshore systems based on large floating structures: Challenges and Opportunities for Brazil – PS192
Isabela Corrêa Hillal	A survey of subsea equipment for offshore transmission systems – PS193
Helena Marques Almeida Silva	Simulation of Power Inverters and Controls in Grid-Connected Wind Systems – PS194
Giancarlo Carvalho Prezotto	Methods for analysis and mitigation of resonances in DER-rich distribution systems – PS195

SHORT ORAL SESSION PROGRAMME

TUESDAY, 7 NOVEMBER 2023

0711 - GHG4 (TV4)

GHG Emilio Silva - Luis Fernando Sá

Anderson Soares da Costa Azevêdo	the topology optimization of CO2 labyrinth seal design considering forward and backward incompressible laminar fluid flow regime
André Dantas Freire	Numerical prediction of erosion in labyrinth seals: A Lifespan approach
Ben-hur Martins Portella	Numerical modeling of sources and sinks of greenhouse gases in the Amazon during the CAFE-Brazil experiment
Carlos Eduardo Lino	Topology Optimization Method Applied to the Design of Radial Compressors Considering Turbulent Real Gas Flow Through Fluid-Structure Interaction and Mechanical Fatigue Analysis
Daniela Andrade Damasceno	Computational Design of Nanostructures and Nanofluidic Systems by Coupling Molecular Simulations with Topology Optimization
Diego Hayashi Alonso	Rotating resonance under low density flow for machine rotor topology optimization
Eduardo Moscatelli de Souza	Design of stepped labyrinth seals by topology optimization
Enrique Vilarrasa Garcia	Influence of the SO2 adsorption on CO2 capture from flue gas using 13X zeolite
Jeann César Rodrigues de Araújo	Synthesis and characterisation of nanomaterials for application in nanofiltration membranes and recovery of lithium from produced water – ETE190
Francisco Hélio Alencar Oliveira	GHG reduction through Topology Optimization and Additive Manufacturing

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - SRS5 (TV1)

SRS Edmilson Moutinho dos Santos - Sigmar Malvezzi

Allan Yu Iwama	Ecosystem-based management as an approach to assessing the social-environmental impacts of offshore wind energy – SRS107
Guilherme Porfirio Baccari 08/11	Risk perception associated with Carbon Capture and Storage technology in Brazil: a comparison between experts and non-experts – SRS102
Gustavo Chagas de Morais	Molecularium: Immersive Experiences for Scientific Dissemination – SRS103
Ricardo Pagio Betini 08/11	How can personality influence perception and behavior towards climate change? An exploratory study – SRS104
Miguel Vera Moreno	A Citizen Science Approach to improving public perception of low-carbon society: A Sentiment Analysis – SRS105
Nelber Ximenes Melo	A Philosophical Framework for Sustainable Energy Planning – SRS106
Bruna Eloy de Amorim 08/11	Congress and Energy Transition: How the interests of the oil and gas sector are represented in the Brazilian Legislative – SRS202
Eduardo Guedes Pereira	CCUS: Legal Developments, Policies and Challenges – SRS203
Giovana Ribeiro Turquetti 08/11	Analysing "O Estado de São Paulo's" perspective on Bioenergy & BECCS – SRS204
Karen Mascarenhas	Social Perception and Science Diplomacy on technology transitions towards a low carbon society – SRS205

SHORT ORAL SESSION PROGRAMME
WEDNESDAY, 8 NOVEMBER 2023

0811 - BECCUS3 (TV2)

BECCUS Hamilton Varela – Marcos Buckeridge

Andrieza de Aquino Eslabão	Brazilian Regulation On Beccs: Gaps, References And Relevance
Leandro Francisco de Oliveira	Hormonal signaling network can contribute to design strategies to improve sugarcane growth and yield
Dawany Dionisio	Electrochemical conversion of CO2 into oxalate with negative carbon footprint
Débora Pagliuso	Fingerprinting agro-industrial wastes: a promise for biomaterials
Haline Rocha	CO2 geological storage in the Paraná Basin, Brazil: an integrated assessment of unconventional reservoirs and caprocks
Jessica Santos Rego	CO2 adsorption on representative feldspar mineral surfaces by first-principles calculations
João Vicotr Vilela Cassiano	Water confined by silica Slits
Sabrina Domingues Miranda	The feasibility of carbon capture technologies in wastewater treatment plants in Brazil
Vitor Favaretto Pinoti	Development of CRISPR-based gene editing tools and identification of herbicide resistance endowing target mutations in sugarcane
Verena Mandorino Kaminagakura	Energy generation in microbial fuel cell in the treatment of vinasse, removal of organic matter and nitrogen
Pedro Henrique de Britto Costa	High power density Solid Oxide Fuel Cells on the temperature range of 400-700 oC, an overview – ETE189

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - CCUSS7 (TV3)

CCUS Lucy Gomes Sant Anna – Renato Gonçalves

Dielle Pierotti Procópio	Conversion of CO2 into biopolymers by the regulation of polyhydroxyalkanoate (PHA) biosynthetic pathway using the photosynthetic cyanobacteria Synechocystis sp.
Gabriel Liscia Catuzo	CO2 hydrogenation to higher alcohols using K-promoted Cu-Fe/UiO-66 catalysts
Antonio Carlos Roveda Junior 175	Surface modification of copper electrodes for electrochemical CO2 reduction
Bruna Bacaro Borrego 176	Micractinium sp., mangroves, and biorefineries: A sustainable trio for third-generation ethanol
Aluizio José Salvador 177	Development of a microfluidic device (rock on a chip) compatible with synchrotron techniques for in-situ monitoring of CO2 storage by rocks
Natalia Lima Vergilio	Geochemical Modeling Of Alteration In Pre-Salt Carbonate Reservoir Rocks In Response To Co2 Injection
Paulo Henrique dos Santos Santana	Stability of turbulent oxy-methane flames in an internal recirculation combustion chamber
Pedro Henrique de Paula Sabanay	A spectroscopic study of Superbase-based Deep Eutectic Solvents for CO2 Capture
Iago William Zapelini	Contributions to the lifetime widening of ZSM-5 zeolites in the ETH reaction – ETE191

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - PS10 (TV3)

PS Maurício Salles – Renato Monaro

Beethoven Narváez-Romo	Carbon Emission Reductions In The University Of Sao Paulo's Transportation – Ps196
Felipe Moreira Sallazar	UAV-Assisted Fault Detection in Electrical Distribution Systems: Computational Simulation – PS157
Gabriel de Castro Biage	Cable Parameter Calculation Through the Finite Element Method – PS158
Giovani Giulio Tristão Thibes Vieira	Flexible Solutions to increase the hosting capacity of distributed energy resources – PS159
Guilherme Broslavschi Pereira da Silva	Analyze of the impact of distributed generation capacity for voltage and reactive support in distribution system – PS160
Guilherme Fidelis Peixer	Performance Assessment of Commercial and Innovative Technologies for Hydrogen Liquefaction – PS197
Joelma Perez	Efficient Use Of Ethanol For Producing Hydrogen And Electricity – Ps198
Julio Cesar Camilo Albornoz Diaz	Influence of NiO content on the Morphological and Electrical Properties of GDC-NiO – PS199
Leandro Oliveira Martins	Optimized RED allocation to increase distributed renewable generation hosting capacity – PS161
Luís Felipe Normandia Lourenço	Investigation of offshore transmission technologies on the Brazilian coast applied in oil and gas exploration and (...) – PS162
Maria Laura Viana Bastos	Automated Circuit Construction for Resonance Analysis in Distributed Energy Resource Integration – PS163

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - EnvSG9 (TV4)

EnvSG Suani Coelho – Edmilson Moutinho dos Santos

Alberto Torres Riera Junior	A Machine Learning Force Field for Boric Acid and Water – EnvSG108
Ana Paula Alves Dibo	Addressing Cumulative Impact Assessment into the planning and development of offshore wind farms (...) – EnvSG109
Alexander Turra	Assessment of the environmental and social impact of offshore wind energy ("EnvSoOff") – EnvSG117
Andrea Carolina Gutierrez Gomez	Municipal Solid Waste Potential for Hydrogen Production in the Sao Paulo State – EnvSG110
Carlos Alberto Martins Junior	Adsorption study of H3BO3 in graphene: a computational approach – EnvSG111
Daniela Higgin Amaral	Potential for electricity generation from sustainable forest management residues in Brazilian isolated systems – EnvSG112
Geovanna Paulino Pereira	Winds of the Future: Multidimensional Assessment of Socio-Environmental Impacts in Offshore Wind Farms – EnvSG113
Guilherme de Aquino Fernandes Sousa	How far has the low-carbon energy transition contributed to energy poverty and social exclusion? – EnvSG114
Ricardo Bastos Calabrese	Integration Of Photovoltaic Energy In Urban Planning – Promoting resilience and decarbonization (...) – EnvSG115
Thalles Moreira de Oliveira	Optimization study of blue hydrogen distribution as an alternative fuel to diesel in the State of São Paulo – EnvSG116
Vanessa Pecora Garcilasso	Life Cycle Assessment (LCA) evaluation of the uses of vinasse produced in the Brazilian sugar sector – EnvSG118

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - NBS15 (TV3)

NBS Carlos Cerri – Maurício Cherubin

Lucas Tadeu Greschuk	Soil carbon storage in Brazilian drylands: status, opportunities and challenges
Thamirys Suelle da Silva	Soil Aggregates and Soil Organic Carbon as Quality Indicators in Crop-Livestock- Forest Integration Systems in The Brazilian Semi-Arid Region
Diego Silva Siqueira	Soil regeneration as a climate strategy and regenerative agriculture
Geraldo Lavigne de Lemos	Brazilian regulation on Nature-Based Solutions: relevance, references and gaps.
Giovanna Pereira Correia	Nanotechnology for hydroponic applications: Development of Metal-organic frameworks (MOFs) for nutrient releasing
Henrique Medeiros Vignati	Two worlds, One Goal: A comparative Analysis of Nature-Based Solutions (NBS) from the Oil Sector and the Global perspective
José Igor Almeida Castro	Effects of improved pasture and integrated systemas on soil carbon sequestration in Brasil
Laudelino Vieira da Mota Neto	Soil aggregates and carbon sycling in maize-forage intercropped systems fertilized with nitrogen
Daniel Aquino de Borda	Impact of Converting Pasture Areas into Sustainable Agriculture on Soil Organic Matter Dynamics
Letícia Oliveira Bispo Cardoso	Comparison of microalgal and cyanobacterial hydrolysate for 3G bioethanol production

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - CCUS11 (TV3)

CCUS Cristina Fernanda Alves Rodrigues – Renato Gonçalves

Renata de Toledo Cintra	Artificial photosynthesis reactions exploring mesoscale 3D printed reactors
Rodolfo Lopes Coppo	Cu-loaded Fe_2TiO_5 catalysts on CO_2 reduction
Rosembergue Gabriel Lima Gonçalves	Evaluation of catalysts derived from MgFe-pyroaurite structure impregnated with potassium in the hydrogenation of CO_2
Saulo de Tarso Alves dos Passos	Enhancing Carbonate Formation in Basalts of the Serra Geral Formation
Sergio Brochsztain	Naphthalenediimide-containing metal-organic frameworks for mixed matrix membranes designed for CO_2 separation
Tamara Ramalho Mignoli	Scale-up study of a pressurized reactor for converting CO_2 to methanol
Vinicio Simizu	Tailoring Pd and Fe Catalysts for Ethanol Synthesis in CO_2 Hydrogenation
Vinícius da Costa Santos	Synthesis of ammonium perrhenate supported catalyst

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - PS16 (TV4)

PS Maurício Salles – Renato Monaro

Marcel Augusto Alvarenga Viegas	Smart and Sustainable Electric Vehicle Fast Charging Station – PS139
Matheus Batista Cordeiro de Souza	Parametric study of an ethanol-based solid oxide fuel cell – PS140
Muhammad Zubair	Cost Modelling of LFAC Transformers: Insights and Implications – PS141
Rafael Braghieri Menillo	Themes and perspectives in Agri-PV research: a global bibliometric analysis showcasing its relevance and importance to energy transition – PS142
Rafael dos Santos Domingues	Li+/Na+ Separation on Production Water using 2D Materials – PS143
Rooney Ribeiro Albuquerque Coelho	Real time monitoring of submarine transmission systems in offshore applications – PS144
Sergio Luciano Avila	Wind turbine diagnostics based on current signatures: a review – PS145
Thiago de Melo Augusto	SOFC – The future of Ethanol in the Transport sector – PS146
Vinícius Soares de Mello Cerqueira	Python Tool for Cost and Loss Analysis in Offshore Energy Transmission – ´S147
Washington Santa Rosa	Processing of ceria-based oxides for use as electrolyte in a solid oxide fuel cell – PS148
Yuri Dionisio de Souza	Algorithm for Fault location of onshore wind farm collector network based on artificial intelligence (“faultAIfinder”) – PS149

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - NBS17 (TV1)

NBS Carlos Cerri – Maurício Cherubin

Bruna Emanuele Schiebelbein	Status of soil health in agricultural soils in Brazil using the Soil Management Assessment Framework
Danielle Mendes Thame Denny 2	Nature-based solutions: Sustainable development of Latin America
Mara Regina Moitinho	Spectral signature of synthetic Fe-rich nanoparticle in an agricultural soil
Marcelo Laranjeira Pimentel	Integrated crop-livestock systems and well-managed pasture promote biological activity, aggregates stability and the increase of soil organic carbon in southern Amazon, Brazil
Márcio José Teixeira	Deforestation Patterns Evolution of the Amazon Basin from 1985 to 2021
Melida del Pilar Anzola Rojas	Potential of Hydrogen Production in Aa Microbial Electrolysis Cell From Sugarcane Vinnasse
Victória Santos Souza	Nature based solution: cover crops in the Cerrado and their role in greenhouse gas emissions and soil carbon distribution
Wanderlei Bieluczyk	On-field measurements of greenhouse gas fluxes in Brazilian low-carbon agriculture: a meta-analysis and critical insights
Danielle Mendes Thame Deny	Connecting carbon farming in Brazil and its implications for food (in)security in África
Dener Oliveira	Make the data available: an analysis of the soil C research for the Brazilian Cerrado
João Luis Nunes Carvalho	Land use intensification as a strategy to increase soil carbon storage and stabilization in tropical conditions

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - PS22 [TV2]

PS Maurício Salles – Renato Monaro

Antônio Carlos Bastos de Godoi	Cyber Defense System for Smart Grid Communications – PS130
Beatriz Aline Riga Rocha	Investigation of Ni and Cu doping effects on the sintering and proton conducting behavior of BaZr0.7Ce0.2Y0.1O3-δ – PS131
Demetrio Cornilios Zachariadis	Wind potential improvement through the study and mitigation of generation deviations and failures – PS132
Carlos Andre Persiani Filho	UAV-Assisted Fault Detection in Electrical Distribution Systems – PS133
Eduardo Coelho Marques da Costa	Parameter estimation of power transmission systems by using least square methods and optimum filtering theory – PS134
Emanuel Percinio Gonçalves de Oliveira	Methodology for Obtaining an Intelligent Tool for Classifying Faults in Overhead and Underground Distribution Lines with High Penetration of Wind Sources Interfaced by Inverters – PS135
Enrique Adalberto Paredes Salazar	Understanding Electrocatalytic Reactions trough Microkinetic Modeling Approaches – PS136
Fátima Eduarda do Nascimento Morais	Methods for the analysis of resonance in distribution systems with high DER penetration – PS137
Felipe Berto Ometto	Catalysts for hydrogen production in ethanol-fed SOEC systems – PS138
Giancarlo Carvalho Prezotto	Methods for analysis and mitigation of resonances in wind farms – PS201

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - CCUS14 (TV2)

CCUS Cristina Fernanda Alves Rodrigues – Pedro Vidinha

Ana Carolina Borges Silva	Particle resolved CFD simulations of fixed bed reactors in co2 hydrogenation
Priscilla J Zambiazi	Engineering porous materials MOFs-Based – Technological Applications and Dynamic Crystals
Andressa Mota Lima 170	Assessment of Non-Aqueous Electrolytes for CO2 Electro-reduction via updated Walden Plot
Bryan Alberto Laura Larico 171	Development of a technical catalyst for the conversion of CO2 into methanol
Alberto Riera J	Lattice Boltzmann methods applied to the solution of Digital Rock problems
Alvaro David Torrez Baptista	Geochemical CO2-basaltic rocks interactions: a first principles approach
Lais Reis Borges	Evaluation of intrinsic catalytic activity of rhenium catalysts at CO2 hydrogenation in a fixed bed reactor during a scale-up process
Lázara Hernández Ferrer	NH3 Production via N2 electroreduction in Water-in-Salt Electrolyte with a MOF Catalyst

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 8 NOVEMBER 2023

0811 - GHG12 (TV4)

GHG Renato Picelli – Fernando Sacomano

Enzo Sampronha	Modeling of Temperature-Swing Adsorption in Fluidized Bed Systems for CO2 Capture
Caroline Silva Matos	Experimental investigations of Brazilian oxygen carriers for the chemical looping combustion technology: from micro- to macroscale
Lucas Neves Braga Soares Ribeiro	Labyrinth Diode Designed by Topology Optimization of Binary Structures using Laminar Flow and Real Gas Properties with Experimental Validation
Juliano Fagundes Gonçalves	Solid Oxide Fuel Cell (SOFC) channel design using the Topology Optimization Method
Marcel Augusto Alvarenga Viegas	Digital Transformation Process Based on Automation and Data Service: a case study in sustainability projects
Thomás C. Miranda	Use of Automated Low-Cost Sensors for Methane (Ch4) Emissions Monitoring
Lucas O. Siqueira	Topology optimization of Turbulent 2D swirl Fluid-Structure Interaction Problems Applied to Labyrinth Seals Design Considering Natural Frequency Constraints
Lucas Ramos Deliberali Barbosa	Decarbonization policies in the industrial sector: a systematic review
Yuri Souza Beleli	Optimization of a continuous temperature swing adsorption system for gases originated from biomass combustion

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 9 NOVEMBER 2023

0911 - ETE6 [TV1]

ETE Virginia Parente – Suani Coelho

Thiago Giancoli Berto	Green and Yellow Hydrogen: from the federal fiscal war to global value chains – ETE119
Melodie Kern Sarubo Dorth Sinegalia	Methodology Proposal for Control Point Surveys: Considerations in the Context of Remote Forest Monitoring with Emphasis on Carbon Stock – ETE120
Mateus Castagnet	Carbon Footprint Reduction through the Replacement of LPG with Biodigesters: A Case Study – ETE121
Leonardo de Freitas	Economic viability of hydrogen – ETE122
Lauron Arend	Business Models for the Brazilian Natural Gas Market in Times of Energy Transition and National Deregulation – ETE123
Jose Roberto Moreira	New Technologies for Cars – Costs, Impacts and Advantages – ETE101
Jhonathan Fernandes Torres de Souza	How much would the energy transition cost for steel and cement industries in Brazil? – ETE124
Felipe Nasser Armond	The Crucial Role of Energy Storage Technologies in the Global Energy Transition – ETE125

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 9 NOVEMBER 2023

0911 - CCUS18 (TV2)

CCUS Lucy Gomes Sant Anna – Pedro Vidinha

Leonardo Domenico De Angelis	Mechanistic insights of the plasmon-enhanced CO2 reduction reaction
Lorenzo Kesikowski Follador	Screening of Ionic Liquids for CO2RR using Molecular Dynamics
Louise Hase Gracioso	Utilizing Microalgae for Sustainable Biorefinery: A Path to Carbon Mitigation and Bioeconomic Prosperity
Luana do Nascimento Rocha de Paula	Effect of the catalyst copper loading on the ethanol production in the CO2 hydrogenation over Cu-UiO-67
Lucas Rodrigues da Silva	Synthesis and Characterization of CuFeZn-based Materials as Catalysts for CO2 Hydrogenation
Maitê Lippel Gothe	Scale up of a ReOx/TiO2 catalyst for the CO2 hydrogenation to methanol
Primaggio Silva Mantovi	Controlling the Role of Water with Ionic Liquids in CO2RR Aiming C2+ Products
Renato Vitalino Gonçalves	Green Hydrogen Production via Photo(electro)catalysis: BiVO4 as case of study

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 9 NOVEMBER 2023

0911 - SRS19 (TV3)

SRS Edmilson Moutinho dos Santos - Karen Mascarenhas

Dindara SIlva Galvão	Future literacy towards climate changes using theater of the oppressed – SRS205
Cylon Liaw	CCUS standardization mapping – The steps towards this strategic tool – SRS206
Celso da Silveira Cachola	Geospatial Analysis and Clustering of Green Hydrogen Production and Consumption for Greenhouse Gas Emission Mitigation: A Case Study of Brazil – SRS207
André dos Santos Alonso Pereira	Science Diplomacy and the Sustainable Development Goals: How RCGI may use it – SRS208
Alberto J. Fossa	Standardization of Carbon Dioxide Capture, Transportation, Utilization and Storage (CCUS) – Recent developments at ABNT and ISO – SRS209
Maxiane Cardoso	Brazilian climate targets and the analysis of their alignment with Nationally Determined Contributions (NDCs) – SRS211
Alexandre de Barros Gallo	GHG mitigation through energy management – Current standardization approaches – SRS212

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 9 NOVEMBER 2023

0911 - GHG20 (TV4)

GHG Renato Picelli – Guenther Krieger Filho

Glycon Pena de Souza Barros	Development of labyrinth seal applied to pneumatic machines using the concept of intelligent materials to minimize leakage
Rômulo Luz Cortez	Compressor's Impeller Designs: Topology Optimization for Resonance Mitigation
Shahin Ranjbarzadeh	Multi-objective function topology optimization design of labyrinth seal
Elóy Esteves Gasparin	Gas-like behavior constraint for s-CO2 Compression Train Optimization
Alberto Lemos Duran	Topology optimization method applied to the design of compressor impellers for supercritical CO2
José Guedes Fernandes Neto	Soil carbon stocks dynamics during tropical forest restoration in Atlantic Forest
Jonatan Ismael Eisermann	Large eddy simulation of a dimethyl ether turbulent jet diffusion flame
João Baptista Dias Moreira	Integer Variable Topology Optimization applied to Full Waveform Inversion for salt reconstruction
Icaro Amorim de Carvalho	Topology optimisation of a rotor subjected to a transient and compressible fluid flow
Teresa Duarte Lanna	Li separation from production water using ZIF-67 – ETE188

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 9 NOVEMBER 2023

0911 - EMS21 (TV1)

EMS Alberto Fossa – Maurício Salles

Andre Luis Ferreira Marques	Solar energy and GHG: a Data Science case study in the Manaus-Parintins Axle – EMS126
João Fegadolli Nunes da Silva	Assessment of Biomethane Potential for Urban Agriculture – EMS127
Letícia Souza de Jesus	Enhancing Predictive Maintenance and Diagnostic Techniques for Stator Fault Detection Using Mathematical Models and Python Simulations – EMS128
Stevan Henrique Ramon de Góes	Using Artificial Intelligence for Image Analysis in Monitoring the Condition of Wind Generator Blades – EMS129

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 9 NOVEMBER 2023

0811 - BECCUS13 (TV1)

BECCUS André Dourado – Marcos Buckeridge

Thiago Vasconcelos de Barros Ferraz	Enabling ethanol electro-oxidation in seawater-like electrolytes for energy conversion and CO2 mitigation
Paula Barione Perroni	Stainless Steel as Catalyst for Ethanol Oxidation Reaction
Naiza Vilas Bôas	The electro-oxidation of ethanol under oscillatory regime on platinum-tin electrodes
Murilo Gomes de Oliveira	Study of Ethanol Electrooxidation in Oscillatory Regime for Gaining Mechanistic Insights.
Marilin Mariano dos Santos	Perspectives of BECCUS technologies in Brazilian sugarcane sector
Leandro Francisco de Oliveira	Hormonal signaling network can contribute to design strategies to improve sugarcane growth and yield
André Henrique Baraldi Doruado	Lignin Oxidation on CuO: (Electro)chemical Approaches
Gustavo Charles Peixoto de Oliveira	Computational Engineering Approaches for Geologic Carbon Storage Site Qualification in the Brazilian
Gabriel Godinho Capistrano	Carbon Capture Utilization and Sequestration in Basaltic Rocks from the Serra Geral Formation: A Petrographic Characterization Before and after the Co2 Injection
Carolina S Costa	Solvent-Free Hydrogenation of Succinic Acid into Tetrahydrofuran

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 9 NOVEMBER 2023

0911 - GHG23 (TV3)

GHG Renato Picelli – Marcelo Sekler

Fernanda de Marco de Souza	GHG emissions in wastewater treatment plants: nitrous oxide and the importance of data collection and monitoring
Felipe Silva Maffei	Design of smart labyrinth seals for mitigation of GHG emissions in pneumatic machines
Emiio carlos Nelli Silva	Design of smart labyrinth seals for mitigation of GHG emissions in pneumatic machines (compressors and turbines)
Renato Picelli	Efficient Turbulent Fluid-Structure Topology Optimization with Smooth Boundaries Using Sequential Integer Linear Programming
Diego Silva Prado	Virtual Analysis Tools for Enhancing Residence Time and Bubble Characteristics in Fluidized Beds
Jurandir Itizo Yanagihara	Design Optimization and Experimental Analysis of Supercritical CO2 Centrifugal Compressors– GHG2013
Daniel Jonas Dezan	Metamodel-Assisted Structural Design Optimization of CO2 Centrifugal Compressor – CCUS215
Maurício Silva Ferreira	Experimental setup for testing supercritical CO2 centrifugal compressors – GHG2014

SHORT ORAL SESSION PROGRAMME

WEDNESDAY, 9 NOVEMBER 2023

0911 - CCUS24 (TV4)

CCUS Lucy Gomes Sant Anna – Renato Gonçalves

Mariana Ciotta	Creating an offshore CCS HUB: challenges and opportunities
Marielle de Oliveira	Design Methodology for Gas-Liquid Separators in Methanol Production from CO2
Daniela Costa 178	The Importance of Reservoir Rocks and Fluids Characterization for Ccs Projects: An Experimental Study With Brazilian Rocks and Fluids
Diego Miranda de Souza Costa 179	Evaluation of the influence of the use of different amino acids and superbases in the preparation of deep eutectic solvents for CO2 capture
Aleksandro Kirch 180	Potential of Clay Minerals for CO2 Capture and Storage: Advances from an Atomistic Perspective
Allan Cavalari Telles Ferreira 181	Challenges to evaluate CO2 storage potential in Saline Aquifers in Brazil
Jose Mateo Martinez Saavedra	Studying the kinetics of CO2 hydrogenation into methanol over commercial copper-based catalysts
Leandro Augusto Faustino	Fine-tuning of electrocatalyst/electrolyte interface for efficient reduction of CO2 and N2 towards added-value chemicals


TV 3

ABSTRACTS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Former Ambassador of Brazil to Japan and India and currently Secretary of Climate, Energy and Environment of Itamar

Energy Transition
RESEARCH & INNOVATION

Research Centre for
Greenhouse Gas Innovation

USP

SHORT ORAL SESSION A

17h20 - Short Oral Session A
0711 – NBS1 (TV1)

Chairs: Carlos Eduardo Pellegrino Cerri – Mauricio Cherubin

Alisson Luiz Rocha Balbino
Universidade de São Paulo

Abstract Title: Exploring Metal Organic Frameworks Synthesis: A Comparative Analysis of Hydrothermal and Mechanochemical Methods

Authors' Names & Affiliation Institutions of all authors (in order for publication): Alisson Luiz Rocha Balbino (IQ/ USP), Giovanna Pereira Correia (IQ/ USP), Priscilla J Zambiazi (IQ/ USP), Dagoberto O Silva (MofTech), Liane Rossi (IQ/ USP).

Abstract: Metal-organic frameworks (MOFs) are crystalline and porous materials formed by the combination of metal centres and organic ligands, gaining prominence in research and practical applications. The flexibility of synthesis conditions affects the morphology, crystallinity, and surface area of MOFs. Conventional methods include solvothermal and hydrothermal approaches. Mechanochemistry, which utilizes mechanical energy to break and form bonds, emerges as a promising alternative, saving solvents and being environmentally friendly. The increasing demand for scalable MOFs makes mechanochemistry attractive, allowing for consistent and efficient production. OPA-MOF, with its role in controlled nutrient release in soil, exemplifies its utility. Studies demonstrate that mechanochemical synthesis significantly reduces the use of reagents, benefiting the environment and the economy. By comparing it to hydrothermal synthesis, this research seeks to determine whether mechanochemistry can produce MOFs equal or superior in structural and functional properties, laying the groundwork for future applications.

Keywords: MOFs, Mechanochemistry, CO2, nutrients delivery.

Introductions and objectives: MOFs are crystalline and porous materials formed by the combination of a metal centre with organic ligands. They represent a remarkable class of materials that have garnered increasing attention in scientific research and practical applications. The versatility in the choice of organic ligands and the metal centre gives MOFs the ability to precisely tailor their properties. Due to their flexibility, synthesis conditions play a crucial role in determining characteristics such as morphology, crystallinity, and surface area of MOFs. In the solvothermal method, an organic solvent is used, and the reaction occurs in a sealed container at high temperature and pressure, promoting the self-organization and crystallization of MOFs. In the hydrothermal method, the reaction takes place in an aqueous

environment with water as the solvent. In addition to these more traditional synthesis methods, mechanochemistry emerges as a promising technique for MOF synthesis, paving the way for a more efficient and sustainable approach. This synthesis method relies on the application of mechanical energy to induce the breaking and formation of chemical bonds, resulting from the high pressure and increased temperature generated by friction. One of the primary advantages of mechanochemistry in MOF synthesis is solvent economy. The absence of solvents makes this process more environmentally friendly, reducing the carbon footprint associated with large-scale production. Anstoetz et al.(2015) described the use of a MOF composed of Fe(III/II) SBUs and phosphate coordinated to oxalate ligands in constructing a 3D porous network containing NH4+ in its pores, resulting in the compound known as OPA-MOF.This porous material is strategically developed to play a crucial role in the controlled release of nutrients into the soil, such as N and P. They also investigated nutrient release performance and the degradation process, revealing that the deterioration of the OPA-MOF structure controlled the gradual release of NH4 and improved soil ecosystem characteristics. The work of Yaxiao et al. (2021) explored the mechanochemical synthesis of this material, demonstrating the feasibility of producing the same MOF with significantly fewer reagents,such as up to a 60% reduction in the use of P sources. This savings benefits not only the environment but also has notable economic implications, highlighting the potential for more sustainable and efficient practices in MOF synthesis. The objective of this study is to establish a comprehensive comparison between mechanochemical synthesis and the conventional process of obtaining OPA-MOF, as reported in the literature through the hydrothermal route. The underlying motivation for this analysis is to determine if mechanochemical synthesis can result in a comparable or even superior material to the MOF produced by the traditional route.

Methodology: The adopted methodology involved the synthesis of the material through both the hydrothermal and mechanochemical routes. The yield was assessed, and the synthesized materials were analysed using spectroscopic techniques, including infrared, Raman, and Mössbauer spectroscopy, along with scanning electron microscopy and X-ray diffraction. Additionally, the surface area and pore volume were characterized using BET (Brunauer–Emmett–Teller) analysis.

Preliminary results: It was possible to synthesize OPA-MOF using both synthesis routes, and the obtained results were in accordance with what is reported in the literature. This confirmation was achieved through the techniques detailed in the methodology. Additionally, the synthesis yield was consistent with expectations. It was possible to synthesize OPA-MOF through both synthesis routes, and the results obtained were in accordance with what is reported in the literature. This confirmation was achieved through the techniques detailed in the methodology. Furthermore, the synthesis yield was consistent with expectations. It is worth noting that the production of the MOF under hydrothermal conditions yields a mass yield of approximately 30%, due to non-reusable residues such as chlorides and phosphates, resulting in a higher synthesis cost compared to that obtained via mechanochemistry. However, the material obtained through mechanochemistry has a chemical yield of 30%, but the mass yield is nearly

95%, allowing for greater utilization of nutrient components for the soil and the advantage of reduced synthesis costs

Preliminary conclusions: This study aimed to synthesize the material through two distinct routes, resulting in MOFs with significant structural differences that can be explored in various applications. The results obtained highlight the mechanochemical synthesis of MOFs as a noteworthy alternative, not only for its eco friendliness but also for the excellent outcomes achieved. This approach allows for parameter adjustments to produce highly customized materials and stands out for its superior yield and ease of production scaling. The MOF synthesized through both routes shows great potential as a natural soil remineralizer, providing controlled release of essential nutrients. This advancement represents a significant step toward more efficient and sustainable agriculture while also underscoring mechanochemistry as a promising alternative in the synthesis of MOFs for diverse applications.

Ana Paula Cervi Ferez
University of Sao Paulo (ESALQ/USP)
RestoreC Project of the NBS Research Program of RCGI - Research Centre for Greenhouse Gas Innovation (PTRB- A1.1)

Abstract Title: Novel field-based models to monitor carbon stocks of forest under restoration in Atlantic forest

Authors' Names & Affiliation Institutions of all authors (in order for publication): Ana Paula CERVI FEREZ1; Pedro Henrique SANTIN BRANCALION2; Otávio CAMARGO CAMPOE3 1 Forestry Engineer, PhD student of the Graduate Program in Forest Resources at University of São Paulo, e-mail: anapaula.ferez@usp.br; 2 Professor at Department of Forest Sciences of University of São Paulo ('Luiz de Queiroz' College of Agriculture – ESALQ/USP); 3 Professor at Department of Forest Sciences of Federal University of Lavras (UFLA)

Abstract: Forest restoration goals are being pledged internationally as strategies for mitigating climate change, although there are still uncertainties regarding the dynamics of carbon storage of restored forests. This work contributes to develop novel models for aboveground biomass (AGB) estimation of forest under restoration to support large-scale recovery of degraded areas. Robust allometric equations will be developed for AGB estimation of forests under restoration. Relations between LiDAR metrics and AGB measurements valued destructively will be evaluated for effective carbon monitoring tool at scale.

Keywords: biomass accumulation; restored forests; remote sensing.

Introduction and Objectives: Monitoring the carbon storage in tropical forests under restoration is crucial to support the ambitious international pledges, but there are still missing

appropriate equations to estimate AGB of forest under restoration. Considering the great biodiversity and complexity of tropical restored forests, it is important to increase the accuracy of AGB estimates. Hence, the development of new reliable methodological approaches to measure carbon stocks is key to endorse forest restoration as a natural climate solution at scale. Remote sensing (RS) has been used to predict AGB in forests, however current methods are based on relations that combine LiDAR-metrics with indirect estimates of AGB, calculated by pantropical equations, non-appropriate for forest restoration areas. The aim of this study is to generate direct estimates of AGB for different forest under restoration (forest plantations and natural regeneration) in the Atlantic Forest, in order to fill the gap of the field-based data used on those RS approaches.

Methodology: Through the destructive method, 80 trees from 20 native species of different sites (SP and BA experimental field trials) will be systemically selected based on the most recent inventory data and sampled to develop site-specific allometric equations for AGB estimation of restored forests. In order to up reach the scale of these critical field-data, we will explore a novel RS methodology that not yet tested in recent research. LiDAR data will be collected from airborne laser scanning (ALS) and terrestrial laser scanning (TLS) assessments in both sites and AGB will be calculated destructively in a 30m x 30m plot (900 m2) in which all trees' individuals present will be sampled. The significance relationships with canopy structure attributes will now be developed using direct measurements of AGB. LiDAR data processing and metrics will be extracted using the LidR package in R. Multiple linear regression analysis will be conducted for adjustment and selection of biomass estimation models (R2, RMSE). Significance correlations with canopy structural attributes will be analysed trough Pearson coefficient. Calibration of the best predictive model for above-ground carbon based on LiDAR metrics based on AIC estimator. The model accuracy will be assessed by leave-one-out cross-validation procedure.

Preliminary results: Development of robust allometric equations to estimate biomass for forest restoration as a function of age and site. Determination of uncertainties in generalist models applied to restoration. Innovative monitoring approach using LiDAR, calibrated with direct biomass measurements. Furthermore, this study will generate a valuable database for further studies relating the AGB of forest landscapes under restoration with canopy structure, accurately provided by remote sensing as LiDAR data.

Preliminary conclusions: It is expected to deepen the understanding of carbon dynamics in different restoration systems aimed at mitigating climate change, which will ultimately allow forest restoration to be effectively implemented as NBS. The results will provide effective at-scale monitoring tool for carbon-targeted forest restoration programs, as well as contribute to the definition of the most cost-efficient forest restoration methods for carbon sequestration in

the Atlantic Forest.

Antonio Yan Viana Lima
Luiz de Queiroz College of Agriculture – University of São Paulo

Abstract Title: Grazing exclusion: a nature-based solution to increase microbial activity in Brazilian desertified drylands

Authors' Names & Affiliation Institutions of all authors (in order for publication): Antonio Yan Viana Lima (Luiz de Queiroz College of Agriculture – University of São Paulo); Arthur Prudêncio de Araujo Pereira (Federal University of Ceará); Maurício Roberto Cherubin (Luiz de Queiroz College of Agriculture – University of São Paulo).

Abstract: Desertification often driven by overgrazing and climate change represents a direct threat to the sustainability of drylands. The need to tackle desertification is crucial to achieving the global environmental goals set by the SDGs. To this end, nature-based solutions such as grazing exclusion are being used to restore desertified areas in Brazilian drylands. Despite this, the effects of grazing exclusion on microbial activity are still poorly understood. This research aimed to evaluate the effects of grazing exclusion on microbial biomass carbon (MBC) content and β-glucosidase enzyme activity in desertified drylands in Brazil. The study was performed in the Desertification Nucleus of Irauçuba (Ceará State) in three sites with two different managements each: i) grazing exclusion for 21 years (RE) and ii) desertified areas by overgrazing (DE), in addition to areas of native Caatinga vegetation (NV) as a control treatment. Soil samples were collected in the 0 - 10 cm layer during the dry and rainy seasons, totaling 54 samples (three sites x three (two managements + one control treatment) x three blocks x two seasons). The analyses were performed in RStudio® software and the significance of the means was tested by Tukey's test ($P < 0.05$). The results showed that the NV and RE areas had the highest MBC contents in the dry season (130.36 in NV and 285.21 mg kg-1 in RE) and in the rainy season (77.71 in NV and 92.63 mg kg-1 in RE), while DE had the lowest contents, regardless of the season (48.08 in rainy and 84.01 mg kg-1 in dry). The same trend was observed for β-glucosidase activity, with the highest activity in the dry season (175.62 in NV and 197.43 mg p-nitrophenol kg-1 solo-1 in RE) and in the rainy season (114.11 in NV and 102.72 mg p-nitrophenol kg-1 solo-1 in RE), while DE showed the lowest activity, regardless of season (37.12 in rainy and 83.09 mg p-nitrophenol kg-1 solo-1 in dry). The increase in SH is driven by the biological balance that occurs through the increase in biological indicators. Grazing exclusion and improving vegetation cover increased soil microbial activity, as observed in our study. RE showed MBC contents and β-glucosidase activity similar to NV and higher than DE, showing that the increase in microbial activity was a response to the increase in vegetation

cover allowed by grazing exclusion.

Keywords: soil quality; biological quality; land degradation; Brazilian semiarid; ecosystem restoration.

Introduction and Objectives: Drylands comprising a sizable portion of the Earth's surface at

41% are confronting substantial environmental challenges, with 10-20% of these regions experiencing degradation. This degradation issue has far-reaching implications, impacting an estimated 250 million people worldwide. In particular, the Brazilian drylands house the most densely populated semiarid region globally is home to approximately 28 million people and, covers roughly 10% of Brazil's total land area. The Brazilian semiarid is characterized by low annual rainfall, resulting in a unique flora adaptation to arid conditions, featuring species such as cacti and thorny shrubs. Unfortunately, intensive human activities like overgrazing have led to a 45% reduction in the native vegetation of the Brazilian semiarid, exacerbating soil degradation and desertification, leading to reduced soil health.

Soil health, defined as the ability of soil to support plant and animal productivity, maintain environmental quality, and contribute to human well-being, is a critical consideration in addressing the multifaceted challenges faced by dryland ecosystems. A comprehensive understanding of soil health in these regions is essential for developing effective strategies to combat degradation, promote sustainable land management practices, and safeguard the livelihoods of the millions of people who rely on these fragile ecosystems for their well-being. Further research is imperative to elucidate the intricate relationships between soil health, land use, and restoration practices within the context of the Brazilian semiarid. Microbial activity in drylands plays a crucial role in the dynamics of ecosystems in these areas. Soil microorganisms play essential roles in decomposing organic matter, cycling nutrients and promoting soil stability. Microbial biomass carbon (MBC) emerges as a key indicator of soil health in dryland environments, reflecting the amount of carbon contained in living soil microorganisms. In addition, β glucosidase enzyme activity, which participates in the carbon cycle and the degradation of recalcitrant organic compounds, plays a key role in the availability of organic carbon for soil microorganisms. In drylands, understanding microbial activity, including MBC and β-glucosidase activity, is fundamental to assessing the resilience and capacity of these ecosystems to cope with environmental pressures and climate change. Therefore, this study aimed to evaluate the effects of grazing exclusion on the microbial activity of soils from long-term restoration areas (21 years of grazing exclusion) in Brazilian drylands, in addition to evaluating the effect of desertification on the microbial activity of soils in drylands. Thus, we hypothesize that (i) grazing exclusion increases the microbial activity of restored soils and (ii) that soils degraded by overgrazing have low microbial activity.

Methodology: The study was conducted in the municipality of Irauçuba, located in the state of Ceará, Brazil, within the experimental research area of the "Irauçuba Desertification Nucleus"

(IDN). This region has a low annual rainfall of approximately 540 mm, which occurs between January and April and has a hot semi-arid tropical climate. The soils in the area are Planosols and, over the last 150 years, livestock activity has led to the removal of the cover and degradation of the soil, including compaction due to grazing and natural factors such as elevated temperatures and water scarcity. The aridity index in the municipality of Irauçuba is 0.26, one of the lowest in the Brazilian semi-arid region. In 2000, experimental areas were established to study the effects of desertification on soil properties, with degraded areas mapped, fenced off to prevent animal access, and left fallow for passive soil restoration. The study was carried out at three sites, each with different land use and management scenarios: 1) native Caatinga vegetation (NV), made up of dry forest fragments; 2) degraded areas (DE) subjected to intensive grazing; and 3) grazing exclusion areas (RE), which were fenced off for 21 years to allow the natural vegetation to recover. Soil sampling was conducted in February 2020 (rainy season) and October 2021 (dry season) in each area, with three replicates established at depth 0-10 cm. Composite samples were sieved (2 mm) and stored at 4 ◦C for biological analyses.

The quantification of MBC followed the fumigation-extraction method, as outlined by Vance et al. (1987) and Polli and Guerra (1997). To assess the potential activity of β-glucosidase (BG) (EC 3.2.1.21), the soil (1 g) was incubated with ρ-nitrophenyl β-glucopyranoside substrate (pH 6.0) at 37°C for 1 hour, and the release of ρ-nitrophenol was measured via spectrophotometry at 410 nm, following the procedure described by Tabatabai (1994). The study assessed homogeneity and normality of variance through the Levene and Shapiro-Wilks tests, respectively. After these initial tests, a pooled analysis using Nested-ANOVA was conducted to comprehend the sources of variability within and between groups. To identify significant mean differences between groups, Tukey's test at a 5% significance level was conducted using RStudio® (Version 1.3.1093).

Preliminary results: The findings indicate notable variations in MBC and β-glucosidase activity across different land use scenarios and seasons. In both the dry and rainy seasons, NV and RE areas exhibited the highest MBC contents, with NV reaching 130.36 mg kg-1 in the dry season and 77.71 mg kg-1 in the rainy season, and RE registering even higher values at 285.21 mg kg-1 and 92.63 mg kg-1 for the respective seasons. In contrast, the Degraded (DE) area consistently showed the lowest MBC levels, with 48.08 mg kg-1 in the rainy season and 84.01 mg kg-1 in the dry season.

A similar pattern was observed for β-glucosidase activity, where NV and RE recorded the highest activities, both in the dry and rainy seasons. In the dry season, NV exhibited β-glucosidase activity of 175.62 mg p-nitrophenol kg-1 soil-1, while RE reached 197.43 mg p-nitrophenol kg-1 soil-1. During the rainy season, these values were 114.11 mg p-nitrophenol kg-1 soil-1 for NV and 102.72 mg p-nitrophenol kg-1 soil-1 for RE. Conversely, the DE area consistently displayed the lowest β-glucosidase activity, with 37.12 mg p-nitrophenol kg-1 soil-1 in the rainy season and 83.09 mg p-nitrophenol kg-1 soil-1 in the dry season. These results underscore the significant impact of land use and management practices on soil microbial parameters, with NV and RE areas exhibiting higher microbial biomass and enzyme activity compared to the DE area, regardless of the season.

Preliminary conclusions: In the context of the restoration areas, the presence of vegetation in Brazil's semiarid emerges as a crucial determinant of soil health, particularly highlighting its positive influence on key soil health indicators such as MBC and β-glucosidase activity. The unique seasonality of the Caatinga biome's deciduous vegetation, marked by significant leaf shedding during the dry season, amplifies biological activity during this period, underscoring the pivotal role of native vegetation in stimulating microbial processes and nutrient cycling in arid environments. This study highlights the importance of employing grazing exclusion as a strategic approach to bolster vegetation cover and improve microbial activity in dryland regions. Furthermore, it emphasizes the sensitivity and rapid response of biological properties as effective indicators for discerning the impacts of detrimental practices on soil health.

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Abstract Title: Carbon stock dynamics in short-term integrated agricultural systems on sandy soils

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Abstract: The conversion of degraded pasture areas to integrated agricultural production systems, such as the crop-livestock-forest system, has been a promising strategy for increasing the carbon (C) stock in the soil and contributing to the reduction of greenhouse gases. As it is a diversified system, there is a greater input of organic material in the soil and also a more diversified input of material. Based on this, the aim was to evaluate the C stock in short-term integrated agricultural production systems in sandy soil. The study was carried out in the municipality of Caiuá/SP with the respective land uses - i. Native forest (MN); ii. Pasture (PA); iii. Crop-livestock integration system with Urochloa brizantha (ILPb); iv. Crop-livestock integration system with Megathyrsus maximus (ILPp).This study investigated carbon (C) stock distribution in different soil layers (0-10 cm, 10-20 cm, and 20-30 cm). In the topsoil layer (0-

10 cm), PA exhibited the highest C stock, likely due to concentrated brachiaria roots, followed by ILPb, while MN and ILPp had lower C stocks. In the subsurface layer (10-20 cm), MN displayed the highest C stock, indicating its ability to store C in deeper soil layers. ILPp also showed significant C stock potential in this layer, followed by ILPb. In the deepest soil layer (20-30 cm), MN again had significant C stock, followed by ILPp and ILPb. Among the integration systems, ILPb had the highest total C stock across all layers (0-30 cm) compared to ILPp. However, differences in soil texture, with ILPb having higher clay content, may influence the stock potential. Importantly, the study found that the three-year period of observation was insufficient for the new integrated systems to surpass the C stock levels observed in stable pastures. This suggests that soil C recovery after pasture conversion may be a slower and more gradual process than initially expected, emphasizing the need for long-term monitoring and management strategies to enhance C sequestration in agricultural systems.

Keywords: soil health, carbon dioxide, greenhouse effect, crop-livestock integration, organic matter.

Introduction and Objectives: Mitigating greenhouse gas (GHG) emissions and climate change has been a major global challenge. Soil is the largest terrestrial compartment of carbon (C) (Kern and Johnson, 1993), and stores around 2,500 Pg C, with 1,500 Pg C in the 0-100 cm soil layer, three times more than is stored in the atmosphere (Machado, 2005; Cias et al., 2013). In recent decades, the world has been discussing the consequences of these impacts on the planet and possible solutions. With the Paris Agreement in 2015 and the United Nations Climate Change Conference (COP 26) in 2021, Brazil committed to reducing greenhouse gas emissions by 37% in 2025 and 50% by 2030 compared to the 2005 baseline (Balau, 2021). Sustainable agricultural development in the country has been the focus of the National Low Carbon Agriculture Plan (ABC Plan) as the main strategy to promote atmospheric C sequestration. One of the GHG reduction strategies developed in the ABC plan is the addition of 5 million hectares of Integrated Agricultural Production Systems (SIPA) (Liell et al., 2018). These systems combine agricultural and/or forestry activities in the same area, with synergies between the components (Balbino et al., 2011). The diversification of the system favors the formation and stabilization of aggregates through which the physical protection of C occurs, added to conservationist management, which maintains the aggregate structure and hinders access to decomposing microorganisms, therefore reflecting on the stock of C in the soil (Lal, 2009). With this in mind, in order to measure the contribution of systems to C sequestration in sandy soil, the following hypothesis was raised: i) Integrated systems, such as crop livestock integration, increase C stock in the short term in sandy soil.

Methodology: The study was carried out in the municipality of Caiuá/SP in the southwest of the state of São Paulo. Located at an average altitude of 375 m, the region has an average temperature of 24.1ºC and an average annual rainfall of 1324 mm, with a tropical climate and a dry winter season (Köppen and Geiger classification). The soil type is Latossolo Vermelho-Amarelo (Santos et al., 2018) with a sandy texture. The area in question was used for livestock

farming from 2007 to 2018, then in 2018 the area was divided to implement the Crop-Livestock Integration System, which was three years old at the time of sampling (February 2022). The study was carried out using the chronosequence of land use change i. Native forest (MN); ii. Pasture (PA); iii. Crop-livestock integration system with Urochloa brizantha (ILPb); iv. Crop-livestock integration system with Megathyrsus maximus (ILPp). In each land use, the soil was sampled to a depth of 30 cm (0-10, 10-20, 20-30 cm) at nine points (repetitions) spaced 50 m apart. The total organic C of each sampled layer was quantified by dry combustion in an elemental analyzer - LECO® CN-2000 (oven at 1350 °C in pure oxygen) and the soil density was calculated by the ratio between the dry soil mass and the ring volume for subsequent calculation of the C stock. Subsequently, the soil C stocks were calculated using the soil density data for this area, using the equation: C stock = C × Ds × Prof where: C stock is expressed in Mg ha-1; C = carbon content in %; Ds = soil density (Mg m 3); Depth = depth of the sampled layer in cm. The C stocks of the different land uses were corrected for equivalent mass, considering the treatment without product as the reference.

Preliminary results: In the topsoil layer (0-10 cm), PA had the highest C stock among the systems evaluated ($p<0.05$), followed by ILPb. This difference suggests that PA was able to accumulate a substantial amount of C in this layer, possibly due to the concentration of brachiaria roots. MN and ILPp exhibited relatively lower C stocks in this layer. The subsurface layer (10-20 cm) revealed a different distribution of C stocks. In this case, MN had the highest C stock, indicating its ability to store C in deeper soil layers, as observed by Costa et al. (2009) in which MN also had low values in the 0-5 cm layer. Notably, the ILPp showed considerable C stock potential in the 10-20 cm layer, followed by the ILPb system. In the deepest soil layer (20-30 cm), MN also stood out with a significant C stock ($p<0.05$), suggesting a continued capacity to sequester C in deeper soil layers. The ILPp and ILPb systems, although they showed lower values compared to MN, still demonstrated considerable C stock potential in this layer. Among the integration systems, Urochloa brizantha (ILPb) was statistically superior to Megathyrsus maximus (ILPp) in terms of total C stock, layer 0 to 30 cm ($p<0.05$). However, it is believed that the textural difference between the soils may be a determining factor in the stock potential, since in ILPb the soil has around 20% clay, while in ILPp the clay content is 11%. However, the results indicate that this three-year period was not sufficient to allow the new integrated systems to surpass the C stock observed in the stable pasture. This suggests that soil C recovery after pasture conversion may be a slower and more gradual process than initially anticipated.

Preliminary conclusions: With the largest amount of C stored among the land uses analyzed, it was observed that this C stock is concentrated in the surface layers of the soil. MN showed greater potential for storing C in deeper layers, even with a sandy-textured soil (10% clay). Due to the recent implementation (three years) in both integrated systems, the C stock was lower compared to the other land uses, so this period was not enough for these systems to surpass the PA stock. Secondly, it was observed that the ILPb system stored more C than the ILPp system. Again, soil texture may have played an important role in this difference in C stock, since ILPb

was in an area with a higher clay content compared to ILPp. These results highlight the complex interaction between soil texture, the time of implementation of the land use systems and the C stock in the soil.

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Abstract Title: Status of soil health in agricultural soils in Brazil using the Soil Management Assessment Framework (SMAF)

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Abstract: Soil provides vital environmental services and plays a central role in achieving the Sustainable Development Goals. However, 40% of the world's soils are degraded, posing a challenge to food production. Soil health, an indicator of a soil's sustainable ecosystem functionality, is critical not only for crop productivity, but also to counter biotic and abiotic stressors. For example, healthier soils have been shown to produce higher yields and be less vulnerable to climate change. - The Soil Management Assessment Framework (SMAF) is one of the most advanced analytical models for assessing soil health. Therefore, the objectives of this work were i) to assess the health of Brazilian agricultural soils using the SMAF tool, and ii) to evaluate differences in soil health at the national scale, using a large set of agricultural data representative of Brazil. To calculate the Soil Health Index for agricultural areas in Brazil, a dataset of 23,997 sample points distributed in 15 Brazilian states and collected in 2021 and 2022 was used. These sample points were obtained from soybean agricultural areas. The SMAF was used to assess soil health at the national level using a minimum data set of five soil health indicators (P, K, pH, Bd and SOC), and the results of the soil health indicators were converted into a score ranging from 0 to 1 (unitless) using algorithms implemented in an Excel® spreadsheet. Finally, the scores for each indicator were integrated into an overall Soil Health Index (SHI) ranging from 0 to 1. The SHI and both indicator scores were interpolated using geostatistical techniques to create a map of spatial variation in soil health and to identify local hotspots of soil health. Exploratory analyses and box plots were performed to evaluate the ISS and score indicators in different biomes and regions of Brazil. The results showed significant

variation in soil health indicators among different Brazilian biomes. In general, the 0-10 cm soil layer is operating at more than 80% of its maximum potential, indicating opportunities to improve soil health through sustainable practices. The SMAF results highlight the inherent influence of climate and soil characteristics on soil health. These findings underscore Brazil's pivotal role in promoting soil health and advancing sustainable agricultural efforts globally.

Keywords: soil quality, soybean croplands, biomes.

Introduction and Objectives: Soil plays a critical role in providing environmental goods and ecosystem services essential for human well-being and achieving the Sustainable Development Goals. However, approximately 40% of the world's soils are degraded, posing one of the greatest challenges to food production. Maintaining and improving soil health is necessary to ensure food security and promote sustainable agricultural development. Globally, the concept of soil health is associated with the continued ability of soil, as a living ecosystem, to perform its functions related to maintaining environmental quality (air and water), promoting human health, and supporting crop productivity. In addition to ensuring crop productivity, healthy soils are critical to reducing crop vulnerability to biotic and abiotic stresses. For example, a recent study in China ((Qiao et al., 2022). found that crops (such as maize, wheat, and rice) grown in healthy soils had higher yields (10.3 ± 6.7%) and lower losses (up to 21%) due to reduced sensitivity to climate variability. Thus, the health of agricultural soils is directly linked to success in addressing major global challenges such as food security and climate change mitigation and adaptation. Due to its broad and complex nature, there is no direct way to measure soil health. Instead, its assessment relies on the integration of chemical, physical, and biological indicators and their interactions. These indicators provide insight into overall soil health, help monitor changes over time, and differentiate between different management practices. With growing global interest and the potential to achieve sustainable development goals through healthy soils, computational approaches have been developed, such as the Soil Management Assessment Framework - SMAF, which is one of the most advanced analytical models. The assessment involves three steps: i) selection of a minimum data set, ii) interpretation of the evaluated indicators, and iii) integration of the indicators into an overall index. In Brazil, several local studies have evaluated soil health using the SMAF tool, highlighting its applicability and sensitivity in distinguishing agricultural crop diversification and land use in the Central South region of Brazil, effects of sugarcane straw removal, agroforestry systems, mangroves, and technosols. Therefore, the objectives of this work were i) to assess the health of Brazilian agricultural soils using the SMAF tool, and ii) to Evaluate differences in soil health at the national scale, using a large set of agricultural data representative of Brazil.

Methodology: To calculate the Soil Health Index for agricultural areas in Brazil, a dataset of 23,997 sample points distributed in 15 Brazilian states and collected in 2021 and 2022 was used. These sample points were obtained from soybean agricultural areas, which include major grain-producing regions. The data were obtained from a large national initiative led by Bayer

S.A. in collaboration with public research institutions, including ESALQ/USP. The SMAF was used to assess soil health on a national scale using a minimum data set of five soil health indicators. The chemical indicators included pH, related to soil acidity, and K and P, related to nutrient cycling, which are key drivers of plant growth and productivity. Bulk density (Bd) served as a physical indicator of soil processes such as aeration, water dynamics, and mechanical resistance to root growth. In addition, soil organic carbon (SOC) was considered a driver of multiple processes and functions, such as nutrient cycling, maintenance of soil structure, and carbon sequestration. These indicators have been widely used in soil health studies both in Brazil and globally. In the second step, the results of the soil health indicators were converted into a score ranging from 0 to 1 (unitless) using algorithms implemented in an Excel® spreadsheet. These scoring curves were specific to each soil type, soil texture, mineralogy, climate, sampling season, slope, crop, and analytical method. In the third and final step, the scores for each indicator were integrated into an overall Soil Health Index (SHI) ranging from 0 to 1 (Equation 1). This value represented the percentage of the total potential functioning of the soil in terms of its ability to perform functions related to crop productivity, nutrient cycling, and environmental protection. SHI has been calculated for 0-10 cm soil depth.

$$SHI = \Sigma Score_i \times Weight_i$$

Where Scorei was the score of the indicator and Weighti was the weighted value of the indicators. The indicators were weighted based on the chemical components (pH, P, and K), physical components (Bd), and biological components (SOC). Thus, regardless of the number of indicators, each group had the same weight (33.33%) in the final index. The SHI and both indicator scores were interpolated using geostatistical techniques to create a map of spatial variation in soil health and to identify local hotspots of soil health.

Preliminary results: Regarding the scores of the chemical indicators, both P and K show similar trends. Scores close to 1 are observed in the Pampa (P: 0.99; K: 0.94) and Atlantic Forest (P: 0.98; K: 0.94) biomes. In contrast, the Cerrado (P: 0.97; K: 0.86) and Amazon (P: 0.97; K: 0.79) biomes recorded lower scores, especially for K. Regarding pH, scores close to 1 were found in the Cerrado (0.93) and Atlantic Forest (0.92) biomes, while the Pampa and Amazon biomes recorded lower values, with values of 0.85 and 0.89, respectively. For soil density, the Pampa had the highest value (0.82), while the Atlantic Forest, Amazon, and Cerrado had lower values of 0.76, 0.76, and 0.73, respectively. For SOC in general, all biomes had scores close to 1 (Pampa -0.98; Atlantic Forest -0.96; Cerrado -0.95; and Amazon -0.88). Finally, in terms of ISS, the Pampa (0.90) and Atlantic Forest (0.88) biomes had the highest ISS scores, compared to Cerrado (0.86) and Amazon (0.83). These results correlate with climatic variables such as temperature and precipitation. The humid subtropical climate (Cfa and Cfb) regulates soil carbon accumulation by slowing the rate of organic matter decomposition and promoting greater plant biomass production. Meanwhile, the presence of highly weathered soils with natural fertility suggests specialized carbon sequestration mechanisms that further enhance carbon storage potential and improve nutrient availability for plants.

Preliminary conclusions: Overall, the 0-10 cm soil layer is operating at over 80% of its maximum capacity across the biomes studied. This suggests that there's still potential to further improve soil health through sustainable management practices. The SMAF tool has proven effective in assessing variation in agricultural soil health in Brazil. However, there's room to refine its interpretation curves by incorporating different soil classes and the diverse climatic conditions found throughout Brazil, which could yield even more accurate results. These results underscore the influence of climate and soil characteristics on SHI and highlight Brazil's unique ability to play a central role in promoting soil health and advancing sustainable agricultural practices on a global scale.

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Abstract Title: Distinguishing microbial pathways responsible for n2o emissions in soils under integrated crop-livestock system

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Abstract: Intensifying agricultural systems by the inclusion of grass species with vigorous root system change the soil physical and chemical attributes and can modify the mechanism of N2O production in soils under integrated crop-livestock (ICL) system. This study is based on the hypothesis that the inclusion of brachiaria grass cultivated with maize modifies soil porosity, the input of organic carbon and nitrogen by roots decomposition and exudation, consequently changing the pathway and intensity of N2O production. The objective of this study was to quantify the contribution of brachiaria on nitrification and denitrification processes to N2O emissions using 15N-labelled fertilizers. A glasshouse study was conducted to understand the 15N-N2O dynamics in soils with and without brachiaria grass. The experimental units consisted of pots with 18 kg of soil on a dry basis. The N fertilizer source was the ammonium nitrate, single (A15N) and double labelled (15A15N). The experiment design was randomized with six treatments and four replicates. The treatments were: 1) Control (soil without plant and N fertilizer); 2) Maize fertilized with 15A15N; 3) Maize fertilized with A15N; 4) Maize + Brachiaria fertilized with 15A15N; 5) Maize + Brachiaria fertilized with A15N. Along the experimental period, soil moisture was adjusted to 60% of the water holding capacity. N2O fluxes were measured during 30 days after fertilization (DAF) until the stabilization of emissions on the control level. The 15N-N2O enrichment was analyzed on an isotope-ratio

mass spectrometer at the University of California, which five time points representing the main N2O emission peaks were chosen. The natural abundance of atmospheric N2O was subtracted from the 15N-N2O enrichment of the samples to calculate the atom % excess. The Maize + Brachiaria significantly boost the N2O production ($p \leq 0.05$) with an emission increase of 78% in comparison to maize monocrop and 85% when compared to the control. The mineral N content presented the same pattern that N2O emissions and in general, high concentration were observed in the first 12 DAF. Regarding the pathways of N2O production, it was observed that the denitrification was responsible for 100% of the N2O emissions 2 DAF in both Maize and Maize + Brachiaria treatments. After that, nitrification was the main N2O production pathway in Maize treatments, contributing with 66%, 69% and 96% of the N2O emissions, respectively to 5, 8 and 10 DAF. On the other hand, changes in the N2O production pathway induced by brachiaria was observed from the 5th DAF, where 89% of N2O came from nitrification. Afterwards the contribution of nitrification decreased to 67% and 30% respectively to 8 and 10 DAF. Our findings confirmed that despite of the high contribution of nitrification process in the tropical soils, the denitrification seems to be equally important during the N2O emission peaks.

Keywords: Greenhouse gas emissions; Root exudates; Soil microbiota.

Introduction and Objectives: Intensifying agricultural systems by the inclusion of grass species with vigorous root system change the soil physical and chemical attributes and can modify the mechanism of N2O production in soils under integrated crop-livestock (ICL) system. In general, the production of N2O in soils occur mainly by nitrification and denitrification pathways, the discrimination between these two routes is a research priority for the establishment management practices mitigating such emissions. Nitrification and denitrification occur in all soils under a variety of abiotic factors such as soil O2 levels, water contents, pH, temperature, NO2- concentrations, organic C contents, inorganic nutrients, availability of C and N, soil disturbance (Hu et al. 2015). In previous studies from subtropical and temperate regions, source portioning of N2O emission using double labelling approach (e.g., 15NH415NO3 and NH415NO3) have identified denitrification process as dominant due to its requirements for available C and N under low pH and low O2 levels found in forests and old grasslands (Russow et al. 2000; Baggs 2008; Morley and Baggs 2010). In tropical conditions, recent studies had indicated that nitrification is the dominant route for N2O production in soils (Soares et al. 2016; Lourenço et al. 2018). To the best of our knowledge, there are no studies evaluating the impacts of the use of brachiaria grasses on the main routes of N2O production in tropical soils using 15N isotope tracer. This technique has been widely applied to discriminate the pathways of N2O emissions by soil 15N enrichment following application of 15N labelled fertilizers/compounds (Baggs, 2008). Based on these statements, we hypothesize that the use of brachiaria in ICL system modify soil porosity and the input of organic carbon and nitrogen by roots decomposition and exudation, and consequently change the pathway and intensity of N2O production in tropical soils. The objective of this study was to apply the 15N approach for the first time to determine the contribution of brachiaria on nitrification and denitrification processes to N2O production using 15N labelled fertilizers.

Specific objectives were: i) Quantify N2O emissions in soil with and without the presence of brachiaria; ii) Discriminate, by isotopic technique, the contribution of nitrification and denitrification pathways to N2O production in soils with and without brachiaria; iii) Evaluate the role of brachiaria root system (biomass and exudates) on N2O production; iv) Correlate the N2O emissions with different soil attributes.

Methodology: A glasshouse study was conducted to understand the 15N-N2O dynamics in soils with and without brachiaria grass. The experimental units consisted of pots with 18 kg of soil on a dry basis. The N fertilizer source was the ammonium nitrate, single (A15N) and double labelled (15A15N). The experiment design was randomized with six treatments and four replicates. The treatments were: 1) Control (soil without plant and N fertilizer); 2) Maize fertilized with 15A15N; 3) Maize fertilized with A15N; 4) Maize + Brachiaria fertilized with 15A15N; 5) Maize + Brachiaria fertilized with A15N. Along the experimental period, soil moisture was adjusted to 60% of the water holding capacity. N2O fluxes were measured during 30 days after fertilization (DAF) until the stabilization of emissions on the control level.

- Gas samplings and analyses

For the GHG quantification, mini static chambers were allocated inside of each experimental unit and closed during the incubation period to gas samplings. Gas samples were collected with syringes after 0,15 and 30 min following chambers closure and then stored in 12 mL pre-evacuated exetainers vials. After all samplings, the chambers were kept open. Concentrations of CO2, N2O and CH4 were measured by gas chromatograph (GC-2014). The CO2 and CH4 gases were detected with FID (flame ionisation detector) and N2O with ECD (electron capture detector). The flux of each GHG was calculated using the linear change in the concentration as a function of the incubation time within the chamber. The 15N-N2O enrichment was analyzed on an isotope-ratio mass spectrometer at the University of California, which five time points representing the main N2O emission peaks were chosen. The natural abundance of atmospheric N2O was subtracted from the 15N-N2O enrichment of the samples to calculate the atom % excess.

Preliminary results: The Maize + Brachiaria significantly boost the N2O production ($p \leq 0.05$) with an emission increase of 78% in comparison to maize monocrop and 85% when compared to the control. The mineral N content presented the same pattern that N2O emissions and in general, high concentration were observed in the first 12 DAF. Regarding the pathways of N2O production, it was observed that the denitrification was responsible for 100% of the N2O emissions 2 DAF in both Maize and Maize + Brachiaria treatments. After that, nitrification was the main N2O production pathway in Maize treatments, contributing with 66%, 69% and 96% of the N2O emissions, respectively to 5, 8 and 10 DAF. On the other hand, changes in the N2O production pathway induced by brachiaria was observed from the 5th DAF, where 89% of N2O came from nitrification. Afterwards the contribution of nitrification decreased to 67% and 30% respectively to 8 and 10 DAF.

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Abstract Title: Nature-Based Solutions (NBS) and the Integration of Local Communities: A Sustainable Path for Socio Environmental Challenges

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Abstract: The sustainable management and utilization of natural resources and processes, known as Nature Based Solutions (NBS), have emerged as a promising strategy to address the socio-environmental challenges currently faced by the world. This academic abstract explores the integration of local communities with Nature-Based Solutions, emphasizing the importance of actively involving communities in the planning and implementation of these approaches. Using a methodological approach that includes literature review and media analysis, we aim to identify the key factors contributing to the engagement of local communities with NBS and their sustainable implementation. Preliminaryy data indicates that the integration of local communities is a crucial element in achieving long-term success and maximizing the benefits of nature-based approaches.

Keywords: Nature-Based Solutions, local communities, sustainability, socio-environmental challenges, natural resources.

Introduction and Objectives: Nature-Based Solutions (NBS) are approaches that seek to address environmental issues such as climate change, biodiversity loss, and ecosystem degradation by utilizing and restoring natural ecosystems. They are relevant for mitigating climate change, conserving biodiversity, and reversing ecosystem degradation, offering additional benefits such as protection against natural disasters and strengthening the resilience of local communities. This study provides a comprehensive view of the importance of NBS and the need to integrate local communities into such initiatives. The objectives of this study are to examine the role of NBS in promoting community integration, identify the key factors contributing to successful integration, and explore the potential benefits and challenges associated with community participation in NBS projects.

Methodology: To achieve these objectives, this study employs a methodology that combines literature review and media analysis. The literature review involves the analysis of academic articles, reports, and case studies related to NBS and community integration. Media analysis focuses on assessing digital and print newspaper articles, social media posts, and other forms of media coverage to gain insights into public perceptions and attitudes towards NBS and community participation.

Preliminary results: Preliminary results highlight that the integration of local communities with Nature-Based Solutions is crucial for the success and sustainability of these approaches. Communities actively involved in the management of natural resources, such as forest restoration, sustainable agriculture, and nature-based water management systems, tend to reap significant economic, social, and environmental benefits. NBS not only help mitigate climate change and conserve biodiversity but also enhance the resilience of local communities in the face of natural disasters. For example, we can cite the "Mangrove Capital Africa" project, led by The Nature Conservancy, which engaged local communities in the restoration of mangroves along the African coast. These communities were trained to plant mangrove seedlings, monitor tree growth, and protect mangroves from harmful activities. Other examples include the "Community-Based Reforestation" project in Indonesia, where local communities restored degraded forests, and the "Agroforestry for Livelihoods" project in Latin America, which promoted agroforestry as a sustainable solution for food production and biodiversity conservation.

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Abstract Title: Integration crop-livestock-forest systems influence soil c stock in the semi-arid of Ceará

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Abstract: Integration of crop-livestock-forest systems (ICLF) can have a positive impact on the carbon footprint, mitigating climate and environmental changes. Therefore, investigating the effects of different ICLF systems on carbon dynamics in the semi-arid can promote the adoption of such strategies in these region. We investigated soil C dynamics in ICLF systems in the semi-arid of Ceará state, Brazil. The study was conducted in an experimental area with four ICLF systems: sorghum (SO), forage cactus (FC), massai grass (MG) and buffel grass

(BG), each with different spacing between native tree strips (NTS) in the Caatinga (7 m – S7, 14 m – S14 and 28 m – S28). These systems were compared with an area of native vegetation (NV) and also with NTS. Soil samples were collected to a depth of 50 cm and soil carbon stocks were determined. Adoption of ICLF systems in NV areas has reduced soil C stocks. However, the C stock lesses varied with species and spacing adopted. Carbon greater loss in the ICLF systems after 6 years occurred in system with forage cactus in S28, while the lower loss occurred in the systems with massai grass and buffel grass, also in S28. The results of the present study provided information on how C dynamics in the soil were influenced to the different spacing adopted between tree strips in ICLF systems in Caatinga.

Keywords: soil organic matter; soil quality; Caatinga.

Introduction and Objectives: Climate change has global implications, and reducing greenhouse gas (GHG) emissions presents a significant challenge. In Brazil, the land use change and agriculture sectors actively contribute to emissions in the country, making it evident, therefore, the need for actions that promote GHG mitigation in these sectors. Soils accumulate three times more carbon (C) than the atmosphere and terrestrial vegetation. Thereby, this large organic carbon pool play a very important role in the global C cycle. One of the strategies to soil organic carbon (SOC) accumulation is conversion of conventional agricultural systems to sustainable production systems. However, in Brazilian semi-arid the predominant land use system in the region is still the conventional one, which begins with cutting and burning of native vegetation followed by the establishment of annual crops along with livestock, with irregular fallow periods. It is also usual for cattle to graze in agricultural fields after harvest, as well as in fallow areas, further reducing the biomass contribution in the region resulting in SOC deficit. Integration crop-livestock-forest (ICLF) systems has been proposed as a promising approach for SOC accumulation and, consequently, to mitigate GHG emissions which are directly associated with global climate change. Is a production system that integrates agricultural, livestock and forest components in rotation, intercropping or succession, within the same production area and which search synergistic effects between the components.
Thereby, understanding the dynamics of SOC in different ICLF systems is essential for the adoption of management strategies that minimize C losses and the release of greenhouse gases. However, in Brazilian semi-arid, agricultural areas with integrated systems, as well as studies which understanding the dynamics C in these systems are still scarce. Therefore, the objective of this study was evaluating the impacts caused on the soil C stocks in ICLF systems in the semiarid of Ceará state, Brazil.

Methodology: The experiment was installed in an experimental area at the Teaching, Research and Extension Unit (UEPE) of the Federal Institute of Science and Technology of Ceará (IFCE), Campus Limoeiro do Norte (05°10′53″ S, 38°00′43″W, 146 m asl), in Limoeiro do Norte, Ceará state, Brazil. The soil was classified as an Cambisol. Climate of the region is characterized by hot and semi-arid, classified as BSw'h according to Köppen-Geiger. The experimental area had

four ICLF systems with different spacing arrangements of natural Caatinga trees (woody component) with dimensions of 6.0×100.0 m, positioned in the north–south direction. The ICLF system was implemented in 2015, using a tractor with frontal blade, suppressing 100% of the vegetation of the cultivable area (understory), directing the residual material to the edges. Before thinning, the experimental area was composed of native arboreal Caatinga. The treatments were: sorghum (SO), forage cactus (FC), massai grass (MG) and buffel grass (BG), each with different spacings (at 7 m – S7, 14 m - S14, and 28 m – S28) between native tree strips (NTS) in the Caatinga and an area of native vegetation (NV). The woody covers 46.15, 30.00 and 17.64% were obtained considering 6.0 m of strip with Caatinga trees, for the spacings of 7, 14, and 28 m, respectively. Soil sampling was performed in January 2021. Disturbed samples were collected from the depths of 0–10, 10–20, 20–30, and 30–50 cm, which resulted in a total of 280 samples (4 depths × 5 replicates × 14 treatments). Besides, were collect undisturbed soil samples using Kopeck rings (5 × 5 cm, height × diameter). In the laboratory, the rings were oven-dried at 105 ◦C for 48 h, and soil bulk density (BD) was calculated based on the weight of oven-dried samples and the total volume of the rings. The disturbed samples were air-dried, sieved (< 2 mm), and roots and plant debris were removed. Sub samples from disturbed samples were taken, ground, and sieved (0.25 mm mesh) before total C determination by the dry combustion method using in an automatic nitrogen-carbon analyser (Thermo Scientific, model Delta V Advantage; Milan, Italy). C stocks were calculated by multiplying the C content, soil bulk density and soil layer thickness. To minimize discrepancies in soil density induced by management practices, calculated C stocks were corrected based on soil equivalent mass. ANOVA ($p < 0.05$) was used to test the significance among treatments (i.e., SO, FC, MG, BG, NV and NTS in each spacings S7, S14 and S28) in each soil depth (i.e., 0–10, 10–20, 20–30 and 30–50 cm) and to the cumulative layers (i.e., 0–30 cm and 0-50 cm). When significant, Tukey's test ($p< 0.05$) was applied to compare the means of treatments. All statistical analyses were carried out using R software (R Core Team, 2019).

Preliminary results: Lower SOC content was observed in systems ICLF compared to forest. Overall, SOC content decreased with depth. The most pronounced impacts were observed in the upmost layer (0-10 cm), where differences were observed in all treatments, which presented an reduction ranging from 11% to 38% compared to NV. For the grasses (MG and BG) and FC, both espacing S28 and S14 resulted in lowers loss in SOC levels. For the SO, the lower impact was been in espacing S14. In the deepes layer (30-50 cm), only SO in E14 decresed SOC levels, which presented an decreased from 1.60 g C kg−1. In NTS, SOC content in 0-10 cm layer were similar to NV, but in 10-20 cm layer, SOC loss occurred, which was lower in 16% compared NV.

Adoption of ICLF systems in NV areas has reduced soil C stocks. However, the effects varied according to the species and system spacing. For the 0-30 cm accumulated layer, our results show that the adoption of greater spacing (S28) in the system with FC induced a loss of 2 Mg ha−1 (i.e., 10%), compared to the S7. Conversely, in the system with MG, spacing S28 (32.4 Mh ha-1) produced a 10% increase in soil carbon stock. Likewise, in the system with SO the highest C stock was observed in the S28, with stock the 28.9 Mg C ha-1. In NTS, C stock were

higher in 7% compared with NV. The rate greast of C stock change for the 0–30 cm layer was observed in the PO in the S28 (1.73 Mg ha-1 yr-1). While, rate lowest was observed in MG in the S28 (0.46 Mg ha-1 yr-1). For the 0-50 cm accumulated layer, differences were found only in the systems with PO and SO, where in the system PO the C stock decreased from 37,11 Mg ha−1 under S7 to 32.88 Mg ha−1 under S28. The significant decrease in C stocks in SO was observed when values decreased from 38.50 Mg ha-1 under S7 to 32.88 Mg ha-1 under S14.

Preliminary conclusions: The adoption of ICLF Systems in Caatinga was investigated. The results obtained showed ICLF systems changed SOC accumulation. Overall, integrated farming systems were influenced to the different spacing adopted between tree strips in ICLF systems in Caatinga. Our findings suggest that adoption of greast spacing between NTS caused lower losses in C stocks in the grasses (MG, BG and SO). On the other hand, in forage cactus, losses in C stocks with spacing S28 were higher than S7. Finally, the results of this study can contribute to a estimate of GHG emissions/removals due to ILPF systems in the Caatinga.

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Abstract Title: Projections of sustainable forest biomass demand as energy source in Mato Grosso

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Abstract: This study examined the potential of sustainable forest biomass utilisation as an energy source in Mato Grosso, Brazil, a region renowned for agricultural production. Despite being a significant agricultural contributor to Brazil's economy, Mato Grosso faces an increasing demand for biomass to serve grain drying and energy generation needs, particularly

in the increasing ethanol sector. This study conducted a comprehensive analysis of energy demand, considering both agriculture and forestry scenarios. It forecasts timber demand for grain drying, focusing on soybeans and maize, which are key crops in the region. The projections suggest a requirement of 15,211,819 m3 of wood and 427,298 ha of planted area over the next five years, emphasising the critical role of forest biomass in supporting agribusiness and sustainable energy production. Leveraging forest biomass for thermal and electrical energy aligns with national sustainability goals, including reducing carbon emissions, as outlined in the Paris Agreement and National Policy on Climate Change. Despite these challenges, this study highlights the considerable potential of sustainable eucalyptus plantations in Mato Grosso to meet the energy demands of the ethanol industry and to maintain agricultural production chains.

Keywords: Bioenergy; potential; forestry; wood.

Introduction and Objectives: Brazil is the 4th largest agricultural producer in the world, with soybean, maize, rice, and seed cotton as the main crops. In this scenario, the state of Mato Grosso is the largest agricultural producer in the Central West region, contributing approximately 27% of the country's total grain production. In the forest scenario, the country also stands out with approximately 9.55 million hectares of planted tree crops and an average annual productivity of 36.8 m3/ha. However, the state still has an incipient planted area despite the high demand aimed at serving the agricultural sector for grain drying and energy generation. In this context, the state of Mato Grosso has emerged as an option for investments in commercial reforestation, leveraged mainly by the consumption of biomass to meet the agroindustry's thermal energy demand, especially that of ethanol from maize, a growing sector in this region. This study aimed to develop a projection of forest-based biomass demand as energy source in Mato Grosso. A literature review was conducted to present the use of this biomass in the national and state energy mix, in addition to the energy analysis of the state and its mesoregions. To determine the main uses and possibilities to expand its use in the state, the agricultural and forestry scenarios were evaluated with a focus on energy generation, and based on this information, the projections for timber demand were estimated. Thus, it is intended to collaborate in the promotion of bioelectricity and the use of thermal energy as well as in the development of a public policy to encourage the use of forest biomass in the production of energy in the state of Mato Grosso.

Methodology: For the theoretical evaluation of wood demand, only the main agricultural products that require drying, namely, soybeans and maize, were considered. For this purpose, the existing scenarios were used to produce each type of crop for the next five years.
To calculate the wood demand projection for grain drying, the Annual Average Increase of 35.6 m3.ha.year was used for the dendrometric variable Total Volume with Bark, at 4.5 years; final was adopted equal to 14%, volume of wood for drying soybeans being 0.0218 m3/t and, for

maize, 0.0574 m3/t.

Preliminary results: The scenarios carried out in this work estimate that the demand for forest biomass for the agricultural sector in the next five years will be 15,211,819 m3 of wood and 427,298 hectares of planted area (considering only the already available land, with no deforestation).

Preliminary conclusions: Forest biomass use has increased as a source of thermal and electrical energy that can promote greater sustainability and security of the national electricity mix, thus meeting the targets for reducing Brazil's carbon emissions in the Paris Agreement and meeting the targets set out in the National Policy on Climate Change law.
There are many challenges to the full establishment of sustainable eucalyptus plantations in the state of Mato Grosso. However, its potential is considerable because the use of forest biomass as an energy source is fundamental to the maintenance of other agribusiness production chains, mainly for grain drying. In addition, the expected increase in maize production, aimed at the ethanol market, promotes the forest planting of fast-growing species to produce solid biofuels to meet the thermoelectric demand of this sector.

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Abstract Title: From Vinasse Pollution to Green Resource: Microalgae-Assisted Biomolecule Accumulation and Toxic Compound Removal

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Abstract: Vinasse is a by-product of first-generation ethanol production that is highly polluting due to its toxic composition and large-scale production, which results in 15 liters of vinasse for every liter of ethanol produced. To reuse this waste, biological treatment with microalgae is a viable solution for eliminating toxic compounds present in vinasse and the simultaneous production of biomass and/or molecules of commercial interest. This biomass is produced by fixing carbon dioxide into carbon-storing molecules by converting light energy into water and oxygen. In addition, stress conditions can be applied to stimulate the accumulation of molecules of interest, such as carbohydrates and lipids, which can be used as biofuel feedstocks. Therefore, the aim is to use a high concentration of vinasse as part of the microalgae culture medium and verify the accumulation of molecules. In this study, two stress conditions, culture medium containing 40% of vinasse and 40% of vinasse with 75% nitrate limitation, were tested to evaluate the biochemical composition in terms of carbohydrate production (through acid hydrolysis and HPLC analysis) and lipids (through Nile Red assay) of four microalgae strains isolated from mangrove in Baixada Santista (B7, B9, D4, and MSC4P). Moreover, the removal of toxic metals such as aluminum, copper, and manganese were also evaluated. Growth conditions were maintained at a light intensity of 185 µmol m-2 s-1 for 24 hours daily with 0.04% CO2 bubbling. The results indicated that the 40% of vinasse condition promoted better glucose production and lower lipid production than the 40% of vinasse condition and 75% nitrate restriction. Strain B7 showed better efficiency in glucose production in 10 days (21% w/w) and removal of toxic metals (16.5% Al, 10% Cu, 100% Mn), demonstrating the potential to contribute to CO2 mitigation and removal of toxic compounds present in vinasse, in addition to producing glucose, which could be used for third generation ethanol production.

Keywords: Bioproducts; Mangrove; Phycoremediation; Wastewater.

Introduction and Objectives: Vinasse is a by-product of first-generation ethanol production that is highly polluting due to its toxic composition and large-scale production, which results in 15 litters of vinasse for every litter of ethanol produced. To reuse this waste, biological treatment with microalgae is a viable solution for eliminating toxic compounds present in vinasse and the simultaneous production of biomass and/or molecules of commercial interest. This biomass is produced by fixing carbon dioxide into carbon-storing molecules by converting light energy into water and oxygen. In addition, stress conditions can be applied to stimulate the accumulation of molecules of interest, such as carbohydrates and lipids, which can be used as biofuel feedstocks. Therefore, the aim is to use a high concentration of vinasse as part of the microalgae culture medium and verify the accumulation of molecules.

Methodology: In this study, two stress conditions, culture medium containing 40% of vinasse and 40% of vinasse with 75% nitrate limitation, were tested to evaluate the biochemical composition in terms of carbohydrate production (through acid hydrolysis and HPLC analysis) and lipids (through Nile Red assay) of four microalgae strains (B7, B9, D4, and MSC4P). Moreover, the removal of toxic metals such as aluminium, copper, and manganese were also evaluated. Growth conditions were maintained at a light intensity of 185 µmol m-2 s-1 for 24

hours daily with 0.04% CO2 bubbling.

Preliminary results: The results indicated that the 40% of vinasse condition promoted better glucose production and lower lipid production than the 40% of vinasse condition and 75% nitrate restriction.

Preliminary conclusions: Strain B7 showed better efficiency in glucose production in 10 days (21% w/w) and removal of toxic metals (16.5% Al, 10% Cu, 100% Mn), demonstrating the potential to contribute to CO2 mitigation and removal of toxic compounds present in vinasse, in addition to producing glucose, which could be used for third generation ethanol production.

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Chairs: Colombo Tassinari – Renato Gonçalves

Fagner Rodrigues Todão
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Abstract Title: The Role of N-Doped Carbon Structures in the Thermocatalytic CO2 Hydrogenation over Co/SiO2 Catalysts

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Abstract: In recent years, the escalating global emissions of carbon dioxide (CO2), primarily attributed to the extensive consumption of fossil fuels, has given rise to critical environmental concerns. To address this pressing issue, the conversion of CO2 into valuable chemical compounds has gained prominence as a viable mitigation strategy. Among the various CO2 conversion approaches, the catalytic CO2 hydrogenation has emerged as a versatile and promising option, albeit with challenges related to carbon-carbon coupling and CO2 adsorption. In the present study, we synthesized Co-based catalysts via a wet impregnation process. Different types of characterizations (such as H2-TPR, CO2-TPD, XRD) revealed the influence of nitrogen and carbon species on Co-based catalysts, affecting the dispersion and reducibility of cobalt particles. Furthermore, carbonaceous deposits on the catalysts were assessed through O2-TPO, as well as the impact of potassium on the carbon structures. In catalytic tests, the introduction of potassium (K), nitrogen (N), and carbon (C) into the Co-based catalysts resulted in enhanced CO2 conversion, with a notable shift towards methane (CH4) as the major product. This study underscores the potential of Co-based catalysts enriched with N, C, and K as effective agents in CO2 hydrogenation, offering a pathway towards important products while

addressing the critical challenge of atmospheric CO2 reduction.

Keywords: Co-catalyst, N-doped carbon, CO2.

Introduction and Objectives: In recent years, there has been a substantial increase in global carbon dioxide (CO2) emissions, resulting in a corresponding escalation of adverse environmental consequences. This escalation is primarily attributed to the extensive utilization of fossil fuels. In response to this pressing issue, the conversion of CO2 into valuable chemical compounds has garnered significant attention as a viable mitigation strategy. Among the various chemical transformations of CO2, the catalytic CO2 hydrogenation has emerged as a particularly versatile and promising approach. However, several challenges persist, notably pertaining to the precise control of carbon-carbon (C-C) coupling reactions and the efficient adsorption of CO2 molecules. In the context of this research, we have undertaken the synthesis of catalysts based on cobalt to systematically investigate the factors governing the CO2 hydrogenation process, with the ultimate goal of generating value-added chemical products.

Methodology: The catalysts were synthesized utilizing a wet impregnation process, following the procedure outlined by Stemmler et al. In summary, cobalt(II) acetate tetrahydrate was combined with 1,10-phenanthroline in ethanol and stirred at a rate of 600 revolutions per minute (rpm) for a duration of 1 hour. Subsequently, silica gel was introduced into the mixture, and stirring was continued overnight at ambient temperature without the application of heat. The liquid phase was then subjected to evaporation, resulting in the formation of a solid material, which was subsequently subjected to pyrolysis at 800°C for a period of 2 hours under an inert atmosphere. This catalyst was denoted as "(5wt%Co)1.0(NC)2.0/SiO2". Adhering to a similar methodology, three additional catalysts were prepared as follows: one without the inclusion of 1,10-phenanthroline, designated as "5wt%Co/SiO2"; another without 1,10-phenanthroline but with the incorporation of potassium, designated as "K0.5(5wt%Co)1.0/SiO2"; and finally, one with the simultaneous inclusion of both 1,10-phenanthroline and potassium, designated as "K0.5(5wt%Co)1.0(NC)2.0/SiO2". All synthesized catalysts underwent a comprehensive characterization process encompassing analyses such as H2 temperature-programmed reduction (H2-TPR), O2 temperature-programmed oxidation (O2-TPO), X-ray diffraction (XRD), and CO2 temperature programmed desorption (CO2-TPD). Furthermore, these catalysts were subjected to rigorous testing in the context of CO2 hydrogenation reactions to assess their catalytic performance.

Preliminary results: The reducibility of the metallic species was evaluated through H2 temperature-programmed reduction (H2-TPR). This analysis revealed distinct reduction zones occurring at approximately 350°C (corresponding to the reduction of Co3O4 to CoO) and at 400°C (corresponding to the reduction of CoO to Co0). Notably, K0.5(5wt%Co)1.0(NC)2.0/SiO2 and (5wt%Co)1.0(NC)2.0/SiO2 exhibited broader reduction

peaks, indicating that the incorporation of nitrogen and carbon species onto the Co-based catalysts had the effect of reducing the uniformity of Co particles and enhancing their dispersion within the catalyst matrix. The assessment of carbonaceous deposits on the catalysts was conducted using O2 temperature-programmed oxidation (O2-TPO). K0.5(5wt%Co)1.0(NC)2.0/SiO2 exhibited a primary oxidation peak at a lower temperature compared to (5wt%Co)1.0(NC)2.0/SiO2, implying that the introduction of potassium (K) slightly disrupted the carbonaceous structure. The results of the catalytic tests demonstrated that the inclusion of potassium (K), nitrogen (N), and carbon (C) in the Co-based catalysts led to an increase in CO2 conversion and favored the production of ethanol. Furthermore, the predominant product shifted towards the formation of methane (CH4).

Preliminary conclusions: The substantial accumulation of carbon dioxide (CO2) in the Earth's atmosphere stemming from the prolonged utilization of fossil fuels has created significant and pressing environmental challenges. In this context, our study serves to illustrate that catalysts based on cobalt (Co), with the incorporation of nitrogen (N), carbon (C), and potassium (K), are promising candidates for studying interesting catalytic effects in the process of CO2 hydrogenation.

Jean Castro da Cruz
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Abstract Title: Development of catalytic pathways for CO2 transformation into chemicals and materials

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Abstract: Environmental impacts related to the growing emission of greenhouse gases is a global problem, and studies into capturing, storing and converting CO2 have been increasingly sought after by the scientific and political community. The development of technologies for converting CO2 can contribute to a carbon-neutral route, as well as enhancing its value in chemical products and fuels. The CO2 hydrogenation reaction is a promising route for producing hydrocarbons and higher alcohols (C2+OH). This reaction can take place in two stages, in the first stage CO is formed via the reverse water-gas shift (RWGS) reaction, and in the second stage the CO formed can be hydrogenated and lead to the formation of hydrocarbons/oxygenates via Fischer Tropsch synthesis (FTS). However, for these reactions to take place efficiently and selectively for hydrocarbons or alcohols, it is necessary to have catalytic sites which, in addition to activating CO2, also perform the C-C coupling and do not

dissociate the C-O molecule. It is therefore necessary to study and develop multimetallic systems that contain these abilities. In addition, understanding the relationship between process variables such as space velocity, temperature and pressure and catalytic activity is crucial to the development of a highly selective catalytic system. This project aims to develop Fe-based catalysts with the addition of transition metals (Cu), noble metals (Rh), and alkali metals (K, Na, Cs), using innovative strategies for the synthesis and characterization of nanoparticles.

Keywords: CO2 Hydrogenation, Fe-based catalysts, higher alcohol synthesis

Introduction and Objectives: The catalytic hydrogenation of CO2 to chemical feedstocks has emerged as a promising technology for recycling CO2 emitted from industries. The CO2 hydrogenation to higher alcohols (C2+) is interesting not only because of the high energy density of the products, but also because they can be hydrogen carriers and fuels, as well as precursors for basic chemical products such as olefins and reagents in the preparation of plasticizers and detergents. Various Fe, Rh, Co, and Cu-based catalysts have been investigated to produce higher alcohols, but catalytic systems with high efficiency are still a major challenge. Thus, understanding and developing catalysts with a greater availability of active sites is highly desirable. Fe-based materials, composed of a Fe+3/Fe+2 phase mixture, are responsible for improving CO2 adsorption on the catalyst surface, due to possible oxygen vacancies. Combining Fe with other metals (such as Rh, Pd, and Cu) is an excellent strategy, since Fe has a low ability to activate CO via the non-dissociative route. Pd catalysts supported on Fe2O3 showed a selectivity to ethanol of 97.5%, while only Fe2O3 led to the formation of CO. The results indicate that ethanol synthesis occurs via the CO insertion mechanism, where the Fe2O3 support transforms CO2 into CO via RWGS and Pd contributes to C-C coupling. Cu can improve the catalytic activity of iron-based catalysts, in which the adsorption force, dissociation energy, and hydrogenation of CO2 are modified by the proportion of Cu added. In addition, Cu is known to have a high adsorptive capacity for CO*, which can be hydrogenated to CHO* and subsequently coupled with the CnHx* species adsorbed on the Fe sites to form the C2+ products. In order to understand more about the control of selectivity to C2+ oxygenates, atomic-level studies based on DFT calculations reveal that selectivity-determining steps in CO2 hydrogenation such as the insertion of CO into CHx, and the hydrogenation of CHx species are related to changes in the composition and structure of the material. Copper is a promising candidate for increasing the selectivity of C2+ oxygenates in the presence of Rh; calculations show that a Cu-decorated Rh alloy has significantly lower energy barriers in the CO insertion step compared to Rh surfaces. Thus, it can be seen that there has been a growing interest in and study of CO2 conversion in recent years; however, the selectivity to ethanol obtained is still low, and the routes and active sites required for the hydrogenation of CO2 to higher alcohols are unclear. Once the role of each active phase is understood, it will be possible to optimize the catalyst and the process, selecting the best temperature, pressure, and pre treatment conditions in order to find economically viable catalysts and processes.

Methodology: The catalysts will be electronically and structurally characterized using various techniques such as XAS, DRX, DRIFTS, SEM, TEM, XPS and TGA. The catalytic tests will be carried out in the gas phase under atmospheric pressure conditions in the CatLab equipment, in a fixed bed reactor, which can undergo heat treatments (25 - 1000°C) under different atmospheres (H2, O2, CO2, CH4, C2H4, CO), in their appropriate proportions under a continuous flow (controlled by flowmeters). The effluent gas will be analyzed by a gas chromatograph coupled to a mass spectrometer (GC-MS Agilent). For reactions that require high pressures, such as the direct conversion of CO2 to hydrocarbons and alcohols, the tests can be carried out in Parr-type reactors (Series 5000 Multiple Reactor System), in batch mode; and continuous flow reactions will be carried out in a reaction line with flow controllers (MKS), with the capacity to operate at pressures of up to 30 bar and temperatures of up to 800°C.

Preliminary results: The results are under development.

Preliminary conclusions: After a literature review, it was decided to develop iron-based catalysts modified with Cu and Rh for CO2 hydrogenation to higher alcohols

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Abstract Title: A combined DFT and machine learning study to understand catalyst and solvent effects on the conversion of CO2 into ethanol

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Abstract: The conversion of CO2 into valuable fuels and chemicals has drawn significant attention due to the possibility of tuning the fuel yield and selectivity by changing the catalyst. Over the decades, advances in theoretical and experimental methods have produced a compendium of complex data containing valuable information on materials that can and should be used to optimize reactions. In this work, our approach combines machine learning methods and DFT data to screen catalysts and find the best candidate to use as a catalyst for CO2 conversion. As previously reported, the C-C bond formation represents the pivotal step to obtaining C2+ products of higher commercial interest, such as ethanol.
The C-C bond coupling is usually related to intermediates, such as C* and CO*. The elementary reactions in transforming gaseous CO2 into these intermediates and side reactions can be used

to find the most favorable reaction pathway as theoretical information from each elemental reaction can be found in the literature for many catalysts, making it suitable for building a dataset and train a machine-learning algorithm. Additionally, we performed DFT calculations to improve the dataset, considering catalysts that already showed good experimental results, mixtures of metals and single-atom supported by usual substrates. The selected catalysts will be verified both theoretically and experimentally. Furthermore, we consider the impact of solvent and alkaline metal cations, as they have been previously demonstrated to play an essential role in these reaction pathways.

Keywords: CO2 conversion; C2+ products; ab initio calculations; machine learning.

Introduction and Objectives: The increased CO2 concentration in the atmosphere has caused many issues, including the greenhouse effect, rising sea levels, and ocean acidification. Despite significant efforts having been made over the last decades, CO2 concentration control and efficient conversion remain challenging. Catalytic hydrogenation of CO2 using H2 produced with renewable energy is considered a potential path forward for the sustainable control of CO2 and its conversion into valuable chemicals like lower olefins, higher hydrocarbons, formic acid, methanol, and higher alcohols.

CO2 hydrogenation to products with at least two carbons (C2+) shares many reaction steps during the CO2-modified Fischer-Tropsch synthesis (CO2-FTS) or MeOH-mediated mechanisms. Various catalysts, including metals, metal oxides, metal carbides, and other metal combinations, have been utilized for CO2 hydrogenation to C2+ . Catalyst supports also significantly affect activity and selectivity due to the strong interactions between active phases and the support.

Research using density functional theory (DFT) was conducted on several metallic surfaces to investigate the mechanisms involved in CO2 reduction. The critical intermediates over these catalysts, such as CO*, CH* and CH2* species, were identified. Furthermore, alkaline metals can accelerate the O* release from the surface, enhancing the catalyst stability and promoting the C-C coupling. Computational studies have already identified means of evaluating the efficiency and selectivity of these metals for this type of reaction. In this way, computational methods can indicate potential catalysts not yet experimentally evaluated for CO2 reduction reactions, with the possibility of screening many new metals and their combinations in different proportions, reducing the experimental efforts, costs, and environmental impacts involved. Also, combining DFT and machine learning techniques has been used to explore catalytic processes and reduce computational efforts. Allied with theoretical advances and machine learning, there are growing efforts to create databases with information on common reactions in catalytic processes.

In this project, our approach combines machine learning methods, DFT data from the literature, and data to be calculated to create a theoretical database. The primary aim is to identify promising new catalysts. The database will encompass a wide range of catalyst types, including those with established favorable experimental results, mixtures of metals, common substrates,

solvent effects, and the presence of alkaline metals, which have previously demonstrated their pivotal roles in these reactions. The evaluation criterion for the potential catalyst will be through the reaction energy, seeking the stabilization of the reaction intermediates. For known intermediates like CH* and CO*, side reactions can be used to find the most favorable reaction path to desired products like ethane or unwanted products like methanol.

Methodology: To implement a robust and accurate database, theoretical information on CO2 conversion reactions was initially collected in publicly available repositories such as the Open Catalysis Project, Catalysis.Hub and Open Reaction. Calculations for populating the database are being conducted within the DFT formalism using the Vienna Ab initio Simulation Package (VASP) electronic structure code, using the BEEF-vdw exchange correlation functional, and 500 eV plane-wave cutoff. Gamma-centered k-point meshes of 6 × 6 × 1 were used, with a 0.15 eV Fermi smearing. The PAW method was used to describe the effect of core electrons. Spin-polarized calculations were performed only for alloys containing Fe, Ni, Co, and Mn, allowing magnetic moments to converge during the electronic structure optimization. All structures were relaxed until the forces acting over each atom were smaller than 0.01 eV Å-1. The Climbing Image Nudged Elastic Band (CI-NEB) approach will search transition states along the reaction pathways. The solvent effects will be included using the VASPsol module. The code implementation of this project involves a series of Python code steps to construct a comprehensive database and apply machine learning techniques for CO2 conversion reactions. Initially, the code converts reaction expressions into SMARTS (Simplified Molecular-Input Line-Entry System) notation. This process enables a more effective representation and handling of reactions. The Chem BERT (BERT for chemistry) model converts the SMARTS representation into a form that can be used to train a machine-learning model. This process turns the complex representation of the chemical reaction into a vector of tokens that capture chemical and structural relationships. The generated tokens were used to train a Support Vector Regressor (SVR) to predict properties such as energy.

Preliminary results: In the initial stage, a literature review was carried out to understand the conversion mechanisms of CO2 (g) to C2+. The surfaces of the catalysts to be studied were listed. In this sense, 37 pure metals and semi-metals were considered, and their 25%, 50%, and 75% combinations resulted in 1998 bimetallic combinations. Reactions involving metals supported on substrates have also shown high potential as catalysts. As a result, we are including reactions of metallic atoms on surfaces such as Al2O3, SiO2, ZrO2, TiO2, CeO2, La2O3, MgO, Nb2O5, and carbon derivatives such as graphite. The effect of adding alkali metals and the solvent effect was also considered in constructing the database. By considering these criteria, with the literature review, a database was built with already known elementary reactions, wit approximately 50 thousand reactions. The calculations were started for ten intermediaries listed as necessary to describe a first mechanism route. Currently, calculations for CH* and CH2* intermediates are being processed. We performed some validations using data already reported in the literature. First, the reaction energy on a copper surface (111) was

compared using another computational code and correlation-exchange functional. Our results showed slightly higher energy values.
Based on the initial observations of the DFT calculations, it was possible to confirm the trend observed experimentally where metals such as Fe, Co, and Ni stabilize CH* and CH2* intermediates. In contrast, noble metals do not stabilize them. Moreover, during our screening process, we found other metals not explored for CO2 conversion into C2+, which can stabilize CH* and CH2* intermediates, such as Al, Cr, Hf, Sc, Ta, Tc, V, and W. To be an excellent candidate as a catalyst for CO2 conversion, a good starting point is stabilizing the intermediates before C-C bond formation. However, we must still analyze other parameters, such as H* and O* stabilization, the energetic barrier to C-C bond formation and solvent effects. Although our results are still Preliminaryy, they show this work's higher potential to indicate new catalysts that can be used for CO2 conversion into olefins. To significantly reduce the timescale to scan all possibilities parallel to the DFT calculations, we are building and optimizing a machine learning algorithm to predict the energy of elementary reactions. The finalization of the machine learning algorithm and the DFT calculations is still necessary to point out new catalysts for capturing and using CO2 (g). However, some evaluations and calculations need to be performed.

Preliminary conclusions: Until this moment of the project, we have successfully identified the intermediaries and promising paths for C2+ products in the literature. The DFT calculations for species of a route are already being processed and indicate that little or unexplored metals for converting CO2 (g) are new possibilities for efficient catalysts. The database for training the machine learning model to predict the adsorption energy on metallic surfaces currently comprises approximately 50,000 reactions. The code is in its evaluation stage, where we are seeking the best possible accuracy in predicting the energies of the reaction. In the following stages of the project, the objective is to continue building the database and obtain data for the other routes and mixtures of metals. Additionally, we plan to assess other effects, such as the presence of common supports used experimentally, as well as solvent and ion effects usually present in heterogeneous catalysis and little explored from a theoretical point of view.

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Abstract Title: Exploring the Impact of Various Supports on K-Promoted Molybdenum-Based Catalysts for CO2 Hydrogenation Reaction

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Abstract: CO2 hydrogenation is a key process for reducing CO2 emissions. Ethanol is among the valuable products generated in this reaction, with numerous potential applications. Nevertheless, this reaction involves a complex reaction mechanism, and the choice of the catalyst is crucial for the optimal performance. In this study, we focused on evaluating the performance of K-promoted molybdenum active phase supported on three different materials (SiO2, CeO2, and ZrO2) for CO2 hydrogenation. In general, the primary products formed were CH3OH and CO. Among these materials, the KMoP/ZrO2 catalyst exhibited the highest methanol selectivity (25.2%). This can be attributed to the acid nature of zirconia support, which favors the formation of CHx species on the catalyst surface. Conversely, KMoP/CeO2 exhibited the highest CO formation, likely due to the oxygen lattice mobility inherent to this type of support. In addition, we evaluated the KMoP/ZrO2 at a higher reduction temperature (800°C), leading to the formation of additional products, including ethanol and hydrocarbon such as CH4 and C2+ species. Therefore, both choice of support and reduction temperature plays pivotal roles in determining the production distribution and selectivity of molybdenum-based catalyst in the CO2 hydrogenation.

Keywords: molybdenum; ceria; zirconia; silica; ethanol; reduction temperature; methanol.

Introduction and Objectives: Converting CO2 into high-value products has been considered an excellent alternative for mitigating CO2 emissions and, consequently, environmental damage. One of the main products in focus is ethanol, which can serve as a versatile chemical, an additive in gasoline, a standalone fuel, or be further transformed into various other products. CO2 hydrogenation is one of the promising pathways for ethanol production. Nevertheless, this route is complex and depends on several variables, such as reaction conditions and catalyst. In general, the product distribution encompasses C1 species like CH3OH, CO and CH4, as well as C2+ species such as alkanes, alkenes, and higher alcohols. Thereby, selectivity is governed by the type of C-O activation and how C-C chain growth occurs in the reaction mechanism. To enhance ethanol selectivity, the catalyst composition assumes pivotal significance, as it needs to minimize undesirable parallel reactions, such as the RWGS and the formation of long-chain hydrocarbons. Metals commonly employed as active phases for this reaction include copper, iron, rhodium, zinc, and molybdenum. In this context, we focus on the use of molybdenum due to its high resistance to sulfur and sintering effect, low-cost and its propensity to favor linear alcohol formation. In the literature, the molybdenum has been exploited in various form, such as metallic Mo, MoO3, MoS2, β-Mo2C, and MoP. Additionally, it has been reported that the synthesis of higher alcohols is promoted by the addition of an alkali metal, such as potassium and sodium. These metals, mainly potassium, have the capacity to adsorb CO in a non-dissociative way on the catalyst surface, facilitating its direct hydrogenation into alcohols. Furthermore, in general, these promoters can influence the reaction mechanism by favoring methanol synthesis, carbon chain growth and/or ethanol formation. Specifically concerning molybdenum, potassium has the capacity to alter the valence state of the molybdenum species

on the catalyst surface, thereby increasing ethanol production. The support also plays an important role in CO2 hydrogenation. It can have positive effects on the active phase and/or participate in the reaction, thereby altering the product distribution. These effects include stabilizing the active phase and promoters, facilitating hydrogen/oxygen mobility, exchanging electrons with the metallic sites, modifying dispersion, and improving reducibility. Therefore, our study investigates the activity and selectivity of K-MoP-based catalysts for CO2 hydrogenation using three different supports (CeO2, SiO2, and ZrO2). We aim to evaluate how these supports influence product distribution and catalytic performance in ethanol synthesis.

Methodology: The catalysts were synthesized using the incipient wetness impregnation. Proper amounts of tetrahydrate ammonium molybdate ((NH4)6Mo7O24.4H2O) and ammonium phosphate ((NH4)2HPO4) were impregnated on commercial supports (SiO2, CeO2, and ZrO2). The materials were dried at 120°C in oven for 12h. After that, the resulting material were calcined at 500 °C for 5h. The nominal composition was 10%K-30%MoP/SiO2, 10%K-30%MoP/CeO2, and 10%K-30%MoP/ZrO2. Prior the catalytic test, the materials were reduced at 500°C for 1 h under H2 (20 mL/min). The CO2 hydrogenation reactions were performed in a fixed bed reactor at 300°C, 20 bar, H2:CO2=3, and total flow of 20 mL/min (GHSV = 4000 mL/gcat h). The final products were analyzed with GC-MS from Agilent.

Preliminary results: We tested three different supported catalyst for CO2 hydrogenation at 300°C, 20 bar, and H2:CO2 molar ratio of 3 during 18 h of time on stream (TOS). The results indicated that all catalysts produced methanol and carbon monoxide. The average selectivities were calculated based on the last 5 hours of the experiment. In general, the selectivity for CH3OH was 9.1%, 17.8%, and 25.2%, while the selectivity for CO was 90.9%, 82.2%, and 74.8% for KMoP/CeO2, KMoP/SiO2, and KMoP/ZrO2, respectively. The CO2 conversion of all the catalysts remained below 1%. It is noteworthy that the choice of different supports had an significant impact on the selectivities of CH3OH and CO, which could be attributed to the characteristics of each support. Silica, as support, has an inert character, making it suitable as a reference material to assess the catalytic activity of molybdenum phosphate. In comparison with KMoP/SiO2, catalysts containing CeO2 and ZrO2 as support exibited higher and lower selectivity to CO, respectively. The higher selectivity of ceria-containign catalysts to carbon monoxide can be explained by ceria´s strong ability to donate /exchange to donate/exchange oxygen to the reaction atmosphere. On the other hand, the acid characteristic of ZrO2 supports tends to produce more CHx species, which are subsequently oxygenated to form CH3OH, explaining the higher selectivity. Temperature-Programmed Reduction (TPR) experiments revealed that the ZrO2 supported catalyst exhibited peaks at higher temperatures compared to the other catalysts. Considering this result, we investigated how the reduction temperature influences the performance of KMoP/ZrO2. In a Preliminaryy result, we reduced the catalyst at 800°C under the same total flow. Under this new reduction condition, the catalyst produce not only CO and CH3OH, but ethanol and hydrocarbon, including CH4 and C2+ products. In this condition, the molybdenum may be in the metallic state, potentially contributing to this altered product distribution. An in situ XRD study will be conducted to identify all the phases are

formed during the reduction process and correlate them with the catalytic performance.

Preliminary conclusions: n this work, we investigated the influence of support materials and reduction temperature on catalytic activity in CO2 hydrogenation. We only identify two products: CH3OH and CO, each exhibiting different selectivity patterns depending on the choice of support. Notably, the KMoP/ZrO2 catalyst demonstrated the highest methanol selectivity, making it a strong candidate for catalyst implementation. Furthermore, we observed that subjecting this catalyst to a higher reduction temperature (800°C) resulted in modifications to the catalyst phases. These modifications made it possible for ethanol and hydrocarbon (CH4 and C2+ species) to form during the CO2 hydrogenation.

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Abstract Title: Tuning catalytic hydrogenation of fumaric acid with supercritical CO2 for GBL and THF production

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Abstract: The selective production of products of interest to the chemical industry such as γ-butyrolactone (GBL), tetrahydrofuran (THF), and 1,4-butanediol (BDO) from the catalytic hydrogenation of fumaric acid (FA) is an interesting reaction in the field of biomass valorization. These products can be considered as molecular construction bioplatforms, serving as starting points for numerous synthesis processes. From a green chemistry perspective, water and CO2 would be ideal solvents, although achieving good conversion rates and selectivity in these reaction media can be a challenge for this hydrogenation reaction, even when an appropriate catalyst is employed. In this context, this process was studied using a palladium-rhenium on silica (Pd-Re/SiO2) catalyst. The catalyst was synthesized through sequential wet impregnation and characterized using X-ray diffraction (XDR), temperature-programmed reduction (TPR), inductively coupled plasma (ICP), transmission electron microscopy (TEM), and surface area and pore volume analysis. The products of the reactions were identified using gas chromatography with flame ionization detection (GC-FID) and high-performance liquid chromatography with refractive index detection (HPLC-RID). Supercritical CO2 was employed as the reaction medium for process optimization, varying the pressure between 105-300 bar under temperature conditions of 60-250 ºC. Finally, the solvent was evaluated considering the

reaction selectivity, where methanol was also used under conditions of 60-250 ºC and 10-300 bar. GBL was produced with 89% selectivity under optimized conditions of 188 °C, 41 bar of H2, and 250 bar of total pressure, using water as a solvent. Supercritical CO2 also proved useful in minimizing the production of by-products during the hydrogenation of GBL, increasing the concentration of GBL and succinic acid in the medium. Changing the solvent had a significant effect on product selectivity, favoring specific reaction pathways. The use of MeOH favored the formation of THF, with a selectivity of 83% under conditions of 175 °C and 50 bar of H2. In MeOH, good conversions and high selectivity for THF at low temperatures were observed, achieving 94% selectivity at 120 °C and 50 bar of H2. The addition of CO2 to the medium maximized the selective production of THF while inhibiting by-products of GBL hydrogenation, achieving 97% selectivity for THF under conditions of 175 °C, 50 bar of H2, and 150 bar of total pressure. It was also observed that varying the partial pressure of CO2 combined with reaction temperature allowed for the reaction to occur in one or two phases, resulting in interesting changes in the final product composition in the medium. For example, the reaction in methanol under conditions of 175 °C and 250 bar of total pressure maximized the production of THF, achieving a selectivity of 91.2% in a single phase. These results contribute to the advancement of the study of this process for flow implementation.

Keywords: Fumaric Acid; Sustainable Chemistry; Experimental Design; Palladium-Rhenium; Iridium-Rhenium; Supercritical CO2.

Introduction and Objectives: The essential energy and raw materials for chemical and material production primarily come from fossil fuels such as oil, natural gas, and coal. Although these resources have driven development, they are highly polluting, finite, and unevenly distributed. To address this issue, recent research has focused on cleaner and renewable energy sources, with biotechnology and "green chemistry" standing out. Biomass, a sustainable source of organic carbon, has the potential to replace oil in the production of fuels and chemicals. However, its chemical complexity requires strategies involving simpler biomass substrates as building blocks. Fumaric acid (FA) is an example of a green, renewable, and versatile raw material that can be transformed into various products, including 1,4-butanediol (BDO), gamma-butyrolactone (GBL), and tetrahydrofuran (THF). Its production is increasing in biorefineries, becoming an alternative to petrochemical products. Global markets for FA, BDO, and GBL are expanding. GBL is a crucial industrial chemical used in cleaning products, strippers, and as a precursor for other chemicals. Currently, GBL is produced from maleic anhydride, depending on petrochemical raw materials, making it vulnerable to price fluctuations and environmental impacts. The use of supercritical carbon dioxide (CO2-SC) as a reaction/solvent medium has the potential to enhance the hydrogenation of compounds, providing greater efficiency and selectivity. However, its use with carboxylic acids, such as FA, is an underexplored area. CO2-SC offers advantages such as safety at larger scales, operation under moderate conditions, and environmentally friendly properties. The addition of water to this system can accelerate reactions in which hydrogen is a reactant. Research aims to optimize GBL production from fumaric acid, a renewable resource, using CO2-SC as a solvent. This has

the potential to improve the efficiency and sustainability of GBL production, contributing to the transition to cleaner and renewable energy sources in the chemical industry.

Methodology: The catalyst was synthesized by sequential wet impregnation of PdCl2 and Re2O7 on to SiO2, and characterized using X-ray diffraction (XDR), temperature-programmed reduction (TPR), inductively coupled plasma (ICP), transmission electron microscopy (TEM), and surface area and pore volume analysis. The hydrogenation of fumaric acid (FA) was carried out in a 10 mL batch reactor using a biphasic system. The liquid phase consisted of a 1 mL aqueous FA solution at a concentration of 1 mg/mL, while the gas phase contained 9 mL of H2 and CO2 at various pressures. Prior to introducing H2 and CO2, the reactor was purged with N2 for 5 minutes. In reactions using a mixture of H2O and MeOH as solvents, the FA concentration was 10 mg/mL. After pre-reducing 10 mg of catalyst in situ using H2 at 300 °C, an aqueous FA solution was introduced into the reactor, and exposure to air was prevented. The reactor was pressurized with H2 at 50 °C, then heated to the reaction temperature, followed by pressurization with CO2. The reaction mixture was continuously stirred at 300 rpm for 20 hours. At the end of the reaction, samples from both the liquid and gas phases were collected and analyzed using gas chromatography with flame ionization detection (GC-FID) and high-performance liquid chromatography with refractive index detection (HPLC-RID).

Preliminary results: The products of the reactions were identified using gas chromatography with flame ionization detection (GC-FID) and high-performance liquid chromatography with refractive index detection (HPLC-RID). Supercritical CO2 was employed as the reaction medium for process optimization, varying the pressure between 105-300 bar under temperature conditions of 60-250 ºC. Finally, the solvent was evaluated considering the reaction selectivity, where methanol was also used under conditions of 60-250 ºC and 10-300 bar. GBL was produced with 89% selectivity under optimized conditions of 188 °C, 41 bar of H2, and 250 bar of total pressure, using water as a solvent. Supercritical CO2 also proved useful in minimizing the production of by-products during the hydrogenation of GBL, increasing the concentration of GBL and succinic acid in the medium. Changing the solvent had a significant effect on product selectivity, favoring specific reaction pathways. The use of MeOH favored the formation of THF, with a selectivity of 83% under conditions of 175 °C and 50 bar of H2. In MeOH, good conversions and high selectivity for THF at low temperatures were observed, achieving 94% selectivity at 120 °C and 50 bar of H2. The addition of CO2 to the medium maximized the selective production of THF while inhibiting by products of GBL hydrogenation, achieving 97% selectivity for THF under conditions of 175 °C, 50 bar of H2, and 150 bar of total pressure. It was also observed that varying the partial pressure of CO2 combined with reaction temperature allowed for the reaction to occur in one or two phases, resulting in interesting changes in the final product composition in the medium. For example, the reaction in methanol under conditions of 175 °C and 250 bar of total pressure maximized the production of THF, achieving a selectivity of 91.2% in a single phase.
Preliminary conclusions: The results obtained in this study provided a better understanding of the biomass valorization process through catalytic hydrogenation reactions of biomass-derived

molecules using supercritical CO2 and palladium-rhenium as a catalyst. The use of CO2-SC as a reaction medium facilitated the selective production of economically important products for the chemical industry from the catalytic hydrogenation of fumaric acid (Ac.FUM), acting as a modulator of catalytic properties, similar to the use of the solvent MeOH. Its use promoted the formation of THF as a product.

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Abstract Title: Synthesis of New Polyurethanes from Biomass-derived Monomers

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Abstract: Polyurethanes (PU) are an interesting class of polymeric materials extensively employed in a variety of industries. Conventionally, they are synthesized by the polyaddition reaction between polyols and diisocyanates, typically from petroleum-derived sources. The work presented herein showcases the synthesis of new PU using biomass-derived monomers. Four new diols were obtained in good yields from 5-(chloromethyl)furfural or CMF (an interesting carbohydrate-derived platform molecule) and dithiols. Subsequently, the polyaddition reaction between these new diols and different diisocyanates was carried out employing organocatalysis as an alternative to the conventional tin-based catalysts.

Keywords: Biomass, Polyurethanes, 5-(chloromethyl)furfural.

Introduction and Objectives: Polyurethanes (PU) are an important class of polymeric materials used in several industries as foams, coatings, elastomers, and more. Their synthesis is conventionally performed by the polyaddition reaction between diols and bis-isocyanates monomers in the presence of some catalyst. However, these raw materials are predominantly derived from petroleum-based sources. An alternative approach to prepare these monomers is the use of biomass-derived platforms. For example, 5-(chloromethyl)furaral (CMF), which is easily prepared from fructose, has become an interesting substrate for the synthesis of monomers, fuels, and sustainable chemicals. In this work, CMF was employed as the starting material for the synthesis of new polyurethanes containing sulfur in their structure. Additionally, the polyaddition reaction was studied by employing organocatalysis (for example, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)) as an interesting alternative to the use of tin-based catalysts, which are difficult to remove from the PU and has high costs.

Methodology: Synthesis of PU from biomass-derived monomers Initially, the nucleophilic substitution reaction between CMF and dithiols was carried out in the presence of triethylamine

and tetrabutylammonium iodide giving the corresponding dialdehydes as the key intermediates. Then, these intermediates reacted with sodium borohydride, providing the desired diols. Four new compounds were obtained using this protocol. Subsequently, the polyaddition reaction between these diols was studied using different diisocyanates and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) as the catalyst.

Preliminary results: A new method to synthesize diol monomers, containing sulfur atoms, was developed from fructose. Twelve new polyurethanes were synthesized by the polymerization reaction between these diols and commercially available diisocyanates. All the polymers were well characterized using nuclear magnetic resonance (RMN), infrared spectroscopy (IR), and thermal gravimetric analysis (TGA).

Preliminary conclusions: New protocol for the synthesis of different diol monomers, containing sulfur atoms, was developed under mild reaction conditions from fructose. These diols were also employed for the synthesis of new biobased polyurethanes by the polyaddition reaction with commercially available diisocyanates.

Giovanni Rodrigues Morselli
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Abstract Title: Interactions between CO2 and superbase in ionic liquids probed by vibrational spectroscopy

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Abstract: Alternative solvents are currently being investigated as media to capture and convert carbon dioxide (CO2), given the corrosive, toxic and volatile properties of traditional amine aqueous solutions used in the CO2 scrubbing process. Ionic Liquids (ILs) are a highlighted class of solvents exhibiting properties as non-volatility, non-flammability and a wide solvent capacity. To enhance CO2 capture efficiency, ILs can be functionalized by incorporating task-specific moieties into their molecular structure or by mixing them with a task-specific compound, such as a superbase - a class of reactive nitrogen bases which are unstable in its pure form or in aqueous solutions. Therefore, the main objectives of this work are: to efficiently capture CO2 by functionalizing ILs through the mixture with the superbase DBU (1,8

diazabicyclo(5.4.0)undec-7-ene), to investigate the interactions between functionalized IL and CO2 through vibrational spectroscopy, i.e., Raman and infrared (IR), and to determine the CO2 sorption mechanism. A series of three ILs, 1-ethyl-3-methylimidazolium thiocyanate (EmimSCN); 1-ethyl-3- methylimidazolium bis(flurosulfonyl)imide (EmimFSI); and 1-ethyl-

3-methylimidazolium tricyanomethanide (EmimTCM) were tested at the molar ratio 2:1 (IL:DBU). At ambient conditions, high CO2 sorption capacities were evidenciated for the three mixtures: 120,6; 65,5 and 66,6 mg/g for EmimSCN-DBU, EmimFSI-DBU and EmimTCM-DBU, respectively. When considering the sorption capacities values in the units of mol CO2 / mol DBU, it is found 1,34; 1,39 and 0,84, respectively. In view of the acidic character of CO2, this quasi-stoichiometric values suggests a direct association CO2-DBU playing a major role in the sorption process. This is supported by spectroscopic results where the disappearence of the C=N stretching band of DBU, at 1613 cm-1 in the Raman spectrum, occurs with CO2 sorption. Also, the CO2 bending mode, c.a. 740 cm-1 in the Raman spectrum, is observed for the mixtures of EmimSCN and EmimTCM, and it is expected only when CO2 molecule is strongly interacting with other species.

Keywords: CO2 capture, superbase, vibrational spectroscopy

Introduction and Objectives: Research on carbon dioxide (CO2) capture by condensed-phase systems have been focusing its efforts to develop alternative media showing thermal and chemical stability, non-volatility and more recently, the suitability to convert the gas in situ into high-value-added products. The traditional method to sorb CO2, based on amine aqueous solution, shows drawbacks as degradation, losses caused by volatilization, and reactor corrosion. Ionic Liquids (ILs) and Deep Eutectic Solvents (DESs) have emerged as promising candidates due to its desirable properties.
Ionic liquids are solvents composed uniquely by ions. Deep eutectic solvents comprise a class of solvents that are prepared by the eutectic mixture of a hydrogen bond donor (HBD) with a hydrogen bond acceptor (HBA), and are considered analogous to ILs due to their shared properties. In DESs, there is a significant decrease in the eutectic melting temperature due to the hydrogen bond network formed between its components. The wide range of DESs that can be prepared is due to the enormous number of combinations between HBAs and HBDs, which are being explored for the production of solvents capable of efficiently capturing and converting CO2. In fact, a range of mixtures between ILs and molecular compounds may be classified as DESs, which is the strategy to be followed by this work. A novel approach consists in using superbases – a class of strong nitrogen bases - to prepare functionalized DES for this application, since CO2 exhibits an acidic character. Neat superbases are unstable compounds, so in order to assure its reactivity towards CO2 it is crucial to form a stable mixture. Various reaction pathways may be followed during the reaction between CO2 and superbases, but the main one involves the formation of the carbamate adduct. Although the adduct is dissociable, its formation facilitates the subsequent conversion of CO2. The presence of water in the medium transforms carbamates into bicarbonates and carbonates, which may be undesirable

when aiming to obtain high-value-added products. Despite some interesting results of CO2 capture by functionalized mixtures in the literature, our understanding of the underlying mechanism and interactions remains rudimentary. Therefore, vibrational spectroscopy - Raman and IR - will be utilized to elucidate the nature of the CO2 sorption process in novel mixtures IL-superbase capable of efficiently sorbing substantial amounts of CO2 at ambient conditions.

Methodology: A series of three ionic liquids, 1-ethyl-3-methylimidazolium thiocyanate (EmimSCN); 1-ethyl-3- methylimidazolium bis(flurosulfonyl)imide (EmimFSI); and 1-ethyl-3-methylimidazolium tricyanomethanide (EmimTCM) were tested in mixtures with the superbase 1,8- diazabicyclo(5.4.0)undec-7-ene (DBU) at the molar ratio 2:1 (IL:DBU). The CO2 sorption capacities were determined and the infrared and Raman spectra were obtained for the neat mixtures and CO2-saturated mixtures.

Preliminary results: At ambient conditions, high CO2 sorption capacities were evidenciated for the three mixtures: 120,6; 65,5 and 66,6 mg/g for EmimSCN-DBU, EmimFSI-DBU and EmimTCM-DBU, respectively. When considering the sorption capacities values in the units of mol CO2 / mol DBU, it is found 1,34; 1,39 and 0,84, respectively. In view of the acidic character of CO2, this quasi-stoichiometric values suggests a direct association CO2-DBU playing a major role in the sorption process. This is supported by spectroscopic results where the disappearence of the C=N stretching band of DBU, at 1613 cm-1 in the Raman spectrum, occurs with CO2 sorption. Also, the CO2 bending mode, c.a. 740 cm-1 in the Raman spectrum, is observed for the mixtures of EmimSCN and EmimTCM, and it is expected only when CO2 molecule is strongly interacting with other species.

Preliminary conclusions: The investigated mixtures have demonstrated high efficiency in capturing CO2 at ambient conditions. Aditionally, a strong association between CO2 and the superbase has been evidenciated, which is expected to be stabilized by the ionic liquid, regardless of the anion.

Gabriel Silveira dos Santos
Fundamental Chemistry Department, Institute of Chemistry University of São Paulo.

Abstract Title: Development of new deep eutectic solvents from low molecular mass hyperbranched polyglycerols associated with superbase for carbon dioxide absorption.

Authors' Names & Affiliation Institutions of all authors: Gabriel Silveira dos Santos, Reinaldo Camino Bazito, Fundamental Chemistry Department, Institute of Chemistry University of São Paulo.

Abstract: Intense emissions of gases such as carbon dioxide (CO2) increase the greenhouse effect and affect the Earth's average temperature. Climate changes, ecological imbalances, and other phenomena harmful to the environment can occur due to these temperature variations. A series of strategies, such as carbon capture, are developed to reduce the impacts of these emissions. Deep eutectic solvents (DES) have emerged as environmentally friendly candidates

for CO2 absorption compared to other traditional methods, such as aqueous solutions of ethanolamine and its derivatives and applications with ionic liquids.
DES are liquid mixtures at low temperatures, composed of two or more substances whose molecules interact with each other through hydrogen bonds, providing an intense reduction in the melting point of the mixture. DES precursors can be simple, low-cost substances, generally less toxic to the environment. The reduction in melting point occurs due to the interaction between a hydrogen bond donor (HBD) molecule, such as alcohols, amines and carboxylic acids, and a hydrogen bond acceptor (HBA) molecule, such as organic salts, such as choline chloride (ChCl). To increase the affinity of DES for CO2, other substances can be added to the mixture, and HBD or HBA can be functionalized. Superbases, in general, are known for their affinity with CO2 and have been used in DES formulations from simpler molecules. Larger molecules, such as hyperbranched polyglycerols (PGOH), can be used as HBD due to the high density of functional groups in the polymer chain. PGOH has multiple hydroxyl groups along the chain and is a good option for the synthesis of DES.
This work aims to present the results of the synthesis of DES using low molecular mass hyperbranched polyglycerols as hydrogen donors and choline chloride, among other organic salts, as hydrogen acceptor. Ternary mixtures containing superbases will also be presented to evaluate DES formation and CO2 absorption. The bases used are 1,4-diazabicyclo [2-2-2] octane (DABCO), 1,5- Diazabicyclo(4.3.0)non-5-ene (DBN) and 1,8-Diazabicyclo(5.4.0)undec-7-ene (DBU). CO2 absorption was evaluated by bubbling the samples with pure CO2 and the mass variation was determined using an analytical balance. We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation, hosted by the University of São Paulo (USP) and sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5;2014/50279-4) and Shell Brasil, and the strategic importance of the support given by ANP (Brazil’s National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Keywords: CO2 absorption, deep eutectic solvents, hyperbranched polyglycerol, superbase.

Introduction and Objectives: High levels of carbon dioxide in the atmosphere are harmful to the environment. Therefore, new materials are developed to capture CO2 and reduce its effects on the planet. Deep eutectic solvents are potential candidates for this purpose. They are mixtures formed by two or more molecules that, after interacting with each other, molecularly, have a lower melting point than their precursors. DES can be associated with other molecules to increase their affinity for CO2.

Methodology: Low molecular weight polyglycerols were synthesized via the ring-opening polymerization reaction of glycidol with trimethylolpropane as the nucleus. The salts used were choline chloride, tetrabutylammonium chloride and cetrimonium chloride. The superbases used were 1,4-diazabicyclo[2- 2-2]octane (DABCO), 1,5-Diazabicyclo(4.3.0)non-5-ene (DBN) and 1,8-Diazabicyclo(5.4.0)undec-7-ene (DBU). CO2 absorption was determined by bubbling CO2 gas at ambient pressure in the samples and the mass variation was determined using an

analytical balance.

Preliminary results: In general, the mixtures have relatively high viscosity and good thermal stability. The DES showed different absorption capacities for CO2 during the bubbling experiment. In some cases, the liquid became opaque, whitish and in others, precipitates formed along the DES. Some desorption tests were carried out using nitrogen gas bubbling.
Preliminary conclusions: The different DES mixtures showed different absorption capacities. It is possible to observe the fundamental role of DES that contain superbase in their composition. DES with superbase have greater absorption capacity than those without. There is probably formation of carbonate or carbamide during CO2 bubbling.

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Abstract Title: Optimization Methodology for Local Control for Efficient Integration of Distributed Energy Resources

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Abstract: This research proposal addresses the growing rise of Distributed Energy Resources - Behind the Meter, DER-BTM, focusing on photovoltaic generation, and the resulting operational challenges for the electrical grid. The main objective of the research is to evaluate strategies for optimized local control of photovoltaic converters and energy storage systems, intending to expand both the hosting capacity and the integration of distributed energy resources. The study aims to examine different scenarios, contemplating the hosting capacity of DER-BTM with due consideration of the restrictions imposed by distribution companies.

Furthermore, more comprehensive control solutions will be reviewed, considering technological maturity and capital and operational costs, as reported in the current literature. A methodology will be developed based on the results obtained to explore control strategies to optimize hosting capacity in a test network. The central focus is to analyse how control adjustments can positively impact the integration capacity of distributed energy resources (DERs). It will investigate how to optimize these controls to allocate distributed resources strategically. Therefore, the optimization method used aims to find an optimized local management that maximizes the hosting capacity of the DERs.

Keywords: Distributed Energy Resources, Hosting Capacity, Optimized Local Control, Photovoltaics.

Introduction and Objectives: Incorporating renewable energy sources into the global energy matrix has experienced a notable increase in recent years. The global expansion of the integration of decentralized energy sources, emphasizing distributed generation (DG), finds its justification in the pressing need for compliance with environmental policies, the growing concern about climate change, and technological advances. According to Energy Research Company (EPE) information, the increase in Distributed Energy Resources (DER) is causing a profound transformation in electrical systems. These systems operate predominantly with large-scale resources, resulting in centralized energy generation. This change in the paradigm of the electrical system is driving the need to adopt new approaches in planning the expansion and operation of electrical networks, especially in distribution networks. Despite the advantages, the broad adoption of DER raises concerns about the energy distribution system. This significant integration changes how these systems operate, increasing the complexity of the challenging process of maintaining the network within its operational limits. To realize the gains resulting from incorporating these distributed resources and ensure adherence to the distribution network's energy quality standards, safety, and operational limitations, it is essential to conduct a series of studies to analyse and evaluate different scenarios. This approach will allow the identification of adverse effects arising from this integration and the proposition of viable solutions to adapt and increase the insertion of der in the network. DG is one of the components of a broader set of DERs. Accompanying DG, there are also energy storage systems and fuel cells. In the current context of Brazil, there is a predominance of distributed photovoltaic generation. It is important to emphasize that conventional distribution feeder design practices did not consider the large-scale presence of DER. The maximum capacity of DERs that a given distribution feeder can accommodate without generating technical problems or requiring changes to the infrastructure is called hosting capacity.

Within this context, the need to create methods and tools to assess the accommodation capacity of these feeders is highlighted. Various calculation approaches and tools have been proposed and developed in recent years. This project aims to develop a methodology to investigate strategies for optimized local control of photovoltaic converters and energy storage systems to expand the hosting capacity and integration of DERs.

Methodology: The methodology focuses on situations in which DERs are connected at the end of the meter, being recognized as DER-BTM. The purpose of this methodology lies in developing a strategic control method called DER-SA. This method aims to improve the planned and efficient allocation of DERs. Its primary focus is to expand the hosting capacity of medium voltage power distribution feeders through the optimized local integration of DERs into the system. The optimization will be carried out using specific software and control strategies for photovoltaic converters, considering the predefined test network for the study.

Preliminary results: This study is currently in the Preliminary phase of conducting a literature review, and as of now, it has not generated any Preliminary findings or drawn any initial conclusions.

Preliminary conclusions: This study is currently in the Preliminaryy phase of conducting a literature review, and as of now, it has not generated any Preliminary findings or drawn any initial conclusions.

Lucas Santos Figueiredo
University of São Paulo

Abstract Title: Development of a Type III generator model for electrical resonance studies in wind farms

Authors' Names & Affiliation Institutions of all authors: Lucas Santos Figueiredo, University of São Paulo. Renato Machado Monaro, University of São Paulo.

Abstract: In recent years, the levels of electricity production from wind power generation have been on the rise in Brazil and worldwide. Nevertheless, most electrical power systems need to be more adequately prepared to accommodate the intricacies of technologies employed within the sector. The Doubly Fed Induction Generator (DFIG) has gained widespread adoption due to its inherent advantages, mainly its ability to effectively control speed and power flow. However, the interaction between the DFIG's impedances and the series or parallel compensators within the transmission system can trigger detrimental events that affect the entire network and connected devices. This study is centered on the development of a Type III wind turbine (WT) model, which proves instrumental in investigating
prevention and damping techniques for subsynchronous resonance (SSR) and high-frequency resonance (HFR). Extensive computational simulations of electromagnetic transients are undertaken to comprehend the nature of these events, demanding substantial computational

resources and a highly qualified engineering workforce. The research's primary objectives include mitigating the risk of equipment damage and contributing to potential updates in Brazil's regulatory framework for wind power plant (WPP) implementations, thus ensuring the sustained growth of wind energy generation while safeguarding system reliability and performance.

Keywords: resonance, wind turbine, DFIG, FACTs.

Introduction and Objectives: Over the past two decades, the installed capacity of electrical power from renewable sources has seen a significant increase worldwide. The primary drivers

of this trend are solar and wind-based generations, with the last one being the focus of this research. A commonly used system is the Doubly Fed Induction Generator (DFIG) or Type III Wind Turbine Generator (WTG), which employs electronic converters to ensure maximum power transfer during generation and better frequency control at the system output. However, this type of device can assume negative equivalent resistance for specific frequencies. The interaction between inductive and capacitive loads in the power system leads to resonances, typically damped by loads and devices connected to the grid. However, due to the aforementioned phenomenon, the interaction of the DFIG with compensating devices compromises the damping of these resonances. Two scenarios are studied: weakly damped resonances (WDR) and undamped resonances (UR). The first incident related to resonances was observed in 2009 in Texas and was published by the Institute of Electrical and Electronics Engineers (IEEE) in 2012. Sub-synchronous resonance (SSR) interactions, which are resonances below the system's fundamental frequency, between the equipment of a WPP and the series compensator devices of the connected transmission line reached detrimental levels for the involved electrical system as a whole. On the other hand, high-frequency resonances (HFR) are typically related to shunt compensators. After the events in Texas and other incidents in different WPPs worldwide, both conditions began to be studied through mathematical models that describe the system in the time domain based on simulations that require high computational costs. Even with such efforts, there are no standard techniques for detecting and mitigating the harmful effects of both phenomena on the system. In this context, this work aims to contribute to the search for appropriate solutions to the resonance management problem in wind farms. A WTG Type III model will be developed to help establish systematic methodologies to prevent and mitigate these phenomena. Furthermore, project results will support potential improvements to park connection regulations established by Brazil's National Electric System Operator (ONS).

Methodology: The methodology employed for the project's development entails, commencing from the state-of-the-art, comprehending the operation of Type III wind turbines. Following this, utilizing the computational software Matlab/Simulink, a mathematical model of the generator is simulated in the time domain to explore its interaction with a test grid equipped with compensation devices. Subsequently, a simplified frequency-domain model is crafted

using the OpenDSS software to investigate resonance interactions.

Preliminary results: The project is currently in the literature review phase to comprehensively understand the DFIG system and the impact of resonances on it.

Preliminary conclusions: The project is currently in the literature review phase to comprehensively understand the DFIG system and the impact of resonances on it.

Luís Fernando Nogueira de Sá
University of São Paulo

Abstract Title: Optimizing PEM Fuel Cell Performance with a Pseudo-3D Approach

Authors' Names & Affiliation Institutions of all authors: Luís and Emílio (Department of Mechatronics and Mechanical Systems Engineering of Escola Politecnica); Fereshteh, Thiago, and Julio (Department of Mechanical Engineering of Escola Politecnica).

Abstract: This work presents a pioneering approach to fuel cell optimization that utilizes a cost-effective pseudo 3D multilayered model, enabling concurrent anode and cathode optimization. The model encompasses key equations for electrochemistry, species transport, fluid flow, energy conservation, and membrane water transport, employing a finite element model for efficient computation. Optimization, utilizing the adjoint method with automatic differentiation, focuses on maximizing power generation while ensuring uniform current density distribution. A density-based approach, using a gradient-based interior point algorithm, yields diverse optimized topologies based on different objective weights. Practicality is demonstrated through post-processing and 3D-printing of optimized prototypes, promising enhanced fuel cell efficiency and cost-effectiveness across various industries. Join us at the congress for an in depth exploration of this transformative approach with applications in energy and transportation.

Keywords: Fuel Cell, Topology Optimization, Pseudo-3D, Finite Element

Introduction and Objectives: The increasing demand for clean energy sources has promoted a big endeavor for low-emission and high-efficiency energy-conversion devices, such as fuel cells. The polymer electrolyte membrane fuel cell (PEMFC) fits these demands with a high energy density and practicality, given that it can be used for stationary and portable applications. olymer electrolyte fuel cells are complex, multilayered devices with noticeable variations in

layer thickness. Conducting three-dimensional (3D) simulations of these cells becomes challenging due to the need for an appropriate number of elements to achieve mesh-independent results and accurately represent the physics occurring in each layer.
Recent works implemented a 3D model and a pseudo-3D (P3D) model for a single channel PEMFC. Their results show a good agreement between variable fields and polarization curves while the P3D runs 40 times faster than the complete 3D.
This work proposes the topology optimization of the PEMFC by using a computationally viable pseudo 3D model. To demonstrate the effectiveness of the proposal, various scenarios are analyzed considering a multi-objective function composed of power generation maximization and current density homogenization.

Methodology: A pseudo-3D model is used to perform the topology optimization of the anode and cathode flow fields simultaneously. The model considers all the physics involved, including

electrochemistry, species transport, multiphasic fluid flow, energy conservation, and membrane water transport.

Preliminary results: Optimized topologies regarding the maximization of power generation are numerically compared with a baseline case. Then, the methodology for the post-processing and 3D-printing of a prototype are shown.

Preliminary conclusions: The proposed model considers a multiphase water behavior and has been shown to be an efficient way to solve the fuel cell design problem. The optimization process resulted in a cathode-anode topology pair that has a significant improvement in the current density homogenization.

Luiza Buscariolli
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Abstract Title: Methodologies for Resonance Analysis in Power Systems with Wind Generation

Authors' Names & Affiliation Institutions of all authors: Luiza Buscariolli (UFABC), Ahda Pionkoski Grilo Pavani (UFABC).

Abstract: The connection of wind generation to power systems poses challenges to maintaining the safe operation of these networks. Events reported in different power systems have raised concerns related to the sub-synchronous resonance due to interactions of control loops of the

converters employed in wind power plants with elements of the power grid. The analysis of this phenomenon is complex, as it requires detailed models of the generation plants, including the controls used in both the converters and the plant, including not only the converter and plant level control parameters but also the analysis of operating conditions and possible grid configurations. Additionally, most analyses are carried out using electromagnetic transient simulations (EMT), which are simulations with high computational burden. As the sub-synchronous resonance due to converter-interfaced generation is a relatively recent phenomenon, the current methods still require improvement to be applied in large systems at connection points with multiple plants with generation connected by converters. In this scenario, this project aims to develop methodologies to identify the risk of sub-synchronous resonance in power systems with high penetration of wind generation, for planning or real time operation applications.

Keywords: Resonance, Sub-synchronous oscillations (SSO), Power Systems Stability, Wind Generation.

Introduction and Objectives: Sub-synchronous resonance has been gaining prominence in the technical/scientific community due to occurrences reported in different countries. The phenomenon of resonance due to wind power plants is associated with two situations: 1) the interaction of converter controls with the series compensation of transmission lines and 2) interactions between converter controls in weak networks, that is, networks with low short circuit power. Another relevant point is that the risk of instability due to resonance is impacted, in addition to control parameters and filters, by the operating conditions of the wind plant and network topology [1]. Several events related to the phenomenon have been reported in electrical networks in several countries, and a report was recently published describing the events and highlighting the importance of investigating the causes associated with the phenomenon, as well as mitigation actions [2]. The document, published in 2022, reports events that occurred in the United States, Canada, Australia, China and the United Kingdom, which occurred under specific operating conditions, the risk of which had not previously been assessed or identified. As this is a relatively recent problem (first formally reported in 2009), there is a lack of well-established and well-accepted techniques in the industry to detect and mitigate this phenomenon, both in weak and unstable damping situations. Faced with the challenges related to the integration of generation connected by converters, this paper aims to develop methodologies for stability analysis due to electrical resonance. The specific objectives are: 1) Investigate and identify the main causes of the resonance event and the critical scenarios where such an event can be initiated. 2) Analyze wind farm and electrical system parameters with the greatest impact on resonance risk. 3) Develop methodologies for identifying the risk of resonance in a wind farm, based on the characteristics (topological and operational) of the park and the electrical system to which the park is connected. 4) Develop techniques to mitigate the risk of resonance occurring in a wind farm.

Methodology: The execution of this project is based on the development of models and analysis through computer simulations. The simulations of EMT type in time domain will be carried out in MATLAB, using the SimPowerSystems. In terms of mapping operating conditions, methodologies associated with Artificial Intelligence can be applied to indicate critical conditions for stability due to resonance both for analysis, in the planning phase, and for operation. In the analyses, wind turbines of type 4 will be used associated with the most susceptible or risky conditions for the occurrence of resonance.

Preliminary results: The expected result is the development of methodologies for the analyses of the risk of instability due to resonance in systems with wind generation. At first, type 4 wind turbine will be considered. The propose methodology can then be applied in the planning and operation of the electrical power systems.

Preliminary conclusions: It is possible to verify a growing number of publications proposing the improvement of analysis techniques and identification of instability or oscillations due to resonance caused by generation connected by converters. Information such as wind plant capacity, active power injected by the plant, short-circuit power level of the connection point, line series compensation level and network topology can be used to estimate the risk of system instability. Furthermore, available measurements can also complement this information, both for short-term planning and real-time operation. Once the risk of instability is characterized, actions aimed at minimizing this risk can be taken, such as changing the network topology, switching series compensation capacitors and changing the control mode of wind plants. Unlike, for example, conventional systems, with generation connected by synchronous generators, in which modal analysis is typically used for this purpose, the equations in the state space of converter interfaced generation systems are complex and, for reasons of industrial secrecy, the models provided by manufacturers for EMT-type simulations are closed (or black-box). Another critical condition is related to systems with multiple converters connected, although plants are usually represented by their equivalents, situations in which there are plants with different generators or controls or even different plants connected at a common point of access to the transmission system, they must be represented by more than one equivalent, which can limit the application of well-known mitigation techniques.

Maria Paula de Souza Rodrigues
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Abstract Title: Utilizing MnO2 Nanowires as Cathodes in Sodium-Ion Batteries Employing Water-in-Salt Electrolytes

Authors' Names & Affiliation Institutions of all authors: Maria Paula de Souza Rodrigues (USP), Roberto Manuel Torresi (USP).

Abstract: Sodium-ion batteries (SIBs) are promising prospects for energy storage due to sodium's abundance and electrochemical properties similar to lithium. Nonetheless, the development and implementation of SIBs present certain challenges, and it is necessary to develop highly efficient electrode materials to achieve optimal performance. In this way, we aim at synthesizing MnO2 nanostructures for use as positive electrodes in sodium-ion batteries employing water-in-salt-electrolytes (WISE). The MnO2 synthesized exhibits a nanorod morphology with a thickness of approximately 52 nm. Our Preliminaryy results from charge-discharge galvanostatic experiments showed high coulombic efficiency and an initial storage capacity of 152 mAh g-1.

Keywords: Aqueous electrolytes, sodium-ion batteries, MnO2, nanowires, cathode material

Introduction and Objectives: The extensive use of fossil fuels has a major environmental impact worldwide, making it urgent to employ and further develop environmentally friendly energy sources and energy storage systems. Lithium-ion batteries (LIBs) are widely used in portable devices owing to their high energy density; nonetheless, their high price and scarcity limit their application in large-scale energy storage systems. Consequently, the replacement of LIBs is imminent, and a promising substitute for these systems is sodium-ion batteries (SIBs) due to the abundance of sodium and its similar electrochemical properties to lithium. However, the development and implementation of SIBs present certain challenges. Sodium-ion is larger than lithium-ion, which limits its diffusion during insertion or extraction into/from the host material. Therefore, it is crucial to develop electrode materials with excellent electrochemical properties and capable of hosting Na+ ions in their structure in a rapid and reversible manner. Manganese dioxide (MnO2) emerges as a promising cathode material for SIBs, due to its abundance, high reversible capacity, and facile Na+ diffusion pathways. Although MnO2 has been extensively studied for SIBs, there are few researchers exploring its application in SIBs employing water-in-salt electrolytes (WISE). The advantage of using WISE is its aqueous nature, which is more environmentally friendly when compared to the organic electrolytes extensively used in portable batteries. Therefore, in this study, we synthesized MnO2 nanowires for use as cathodes in sodium-ion batteries employing water-in-salt electrolytes. These nanowires are interesting due to their nano-sized structure, which may facilitate the Na+ diffusion process.

Methodology: MnO2 synthesis followed a procedure from the literature. The electrodes were prepared by dispersing MnO2 nanorods, carbon black and poly(vinylidene fluoride) binder (PVDF) in N-methyl-2-pyrrolidone (NMP) to form a slurry. The resultant slurry was pasted onto a carbon coated aluminum foil using a doctor blade. The electrochemical measurements were carried out using three-electrode Swagelok cells and two electrode coin cells (CR2032-type). In WISE, Pt was used as the reference electrode (for the three electrode cells) and carbon

was used as the counter electrode. In organic electrolytes, sodium was used as both reference (for the three-electrode cells) and counter electrode. A glass microfiber (Whatman) was used as separator in all cases. Cyclic voltammetries and charge-discharge galvanostatic curves were registered.

Preliminary results: We synthesized MnO2 nanorods with a thickness of approximately 52 nm. The XRD and Raman data showed that MnO2 presents an alpha-phase. Galvanostatic charge-discharge curves were registered using a water-in-salt electrolyte and our system showed a high coulombic efficiency with an initial storage capacity of 152 mAh g-1 (0.05C, 15.4 mA g-1).

Preliminary conclusions: MnO2 showed a promising application in SIBs with WISE, nonetheless further studies need to be performed to verify its cyclability and performance when compared to commercial MnO2 and organic electrolytes.

Mário Oleskovicz
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Abstract Title: Fault location of onshore wind farm collector network based on artificial intelligence and drone supervision ("faultAIfinder")

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Abstract: Thus, this research project aims to develop a hybrid system composed of intelligent diagnosis of faults (detection, classification, and location) and drones for aerial supervision. The system is classified as a hybrid because it combines different intelligent techniques to

perform short-circuit diagnosis to exploit the strengths of each one of them, in addition to aerial supervision by drones. Signal pre-processing tools will be investigated for fault detection, classification, and location. Next, some of the techniques based on Artificial Intelligence (AI), such as machine learning, will be evaluated and used to diagnose the fault situation that was faced. In addition, once the fault is located, an aerial drone will be activated to collect images of the exact location of the fault situation. They will be transmitted to the maintenance team for the correct planning of correcting the disturbance in medium voltage aerial feeders. The results of applying the hybrid system will provide greater agility in the fault location process, reducing the downtime of wind farms due to short-circuit shutdowns and providing greater security to the maintenance team.

Keywords: Onshore wind farm; Hybrid system; Intelligent diagnosis of faults; Drones for aerial supervision

Introduction and Objectives: This project's main objective is to develop an efficient system for diagnosing faults in medium voltage feeders of onshore wind farms, with support and refinement of results through images captured by aerial drones. The method to be developed will provide the maintenance team with information about the exact location of the fault and the recognition of the physical elements at the site through high-definition images and thermal images, thus aiming to reduce the time to locate the short-circuit and the unavailability of wind farms.

Methodology: This proposal was planned to be executed in 36 months, considering six main stages, aiming to provide agility during its development. Within each step, intermediate and complementary steps will be carried out simultaneously by different team members who will join in due course. Initially, Stage 1 will have two fundamental activities: computational modeling of the medium voltage overhead and underground power system and the test wind farm for fault diagnosis; and modeling of medium voltage aerial feeders in a virtual environment to simulate drone navigation. In Step 2, from the modeled test system, all scenarios of interest will be generated in an electromagnetic transient simulation program, providing information (data) for the development of fault detection and classification techniques (Step 3) and the AI-based fault location algorithm (Step 4). Next, Steps 3, 4, and 5 will correspond to the development of a large part of the research, having two main work fronts: (1) development of fault detection, classification, and location methods, and (2) development of drone navigation methods and image processing algorithms. Step 6 will comprise tests in a controlled environment of the complete system, that is, the diagnosis of faults in the drone's aerial visualization and navigation system.

Preliminary results: For the moment, the main stages associated with the development of the project concern the literature review concerning the test system to be used, the detection,

classification and location of the fault, and the application of drones in the aerial supervision of electrical power systems. Therefore, the initial results reflect what was found in related literature, focusing on onshore wind farms, and which are related to the previously mentioned steps. However, there are still no conclusive aspects to be reported.

Preliminary conclusions: The initial results reflect what was found in related literature, focusing on onshore wind farms related to the test system to be used, the detection, classification and location of the fault, and the application of drones in the aerial supervision of electrical power systems. Unfortunately, there are still no conclusive aspects to be reported.

Marilin Mariano dos Santos
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Abstract Title: Long-term offshore systems based on large floating structures: Challenges and Opportunities for Brazil

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Abstract: Large floating structures or “Very Large Floating Structures” (VLFS) can be defined as artificially constructed floating structures for the maritime environment. VLFS can be used for the creation of airports, hotels, cities and even for industrial or power generation purposes, through shipping plants to main gas processing plants, or offshore electrical generation. The VLFS structures to be analyzed in this project proposal are designed to be installed in high-depth maritime environments, typical of where the main offshore oil and gas (O&G) exploration and production occurs in Brazil, with specific references to the areas of pre-salt polygon and, particularly, those associated with CNOOC's main O&G producing assets in Brazil, that is, the Búzios and Libra fields. VLFS-type solutions attract the attention of engineers, architects and urban planners because they provide ecological and interesting solutions in the form of creating “habitable areas” in maritime regions. In this research, such solutions are considered in the field of integrated planning for a broader energy, mineral and economic exploration of oceanic resources. VLFS-type structures are then conceived as central elements to compose Greener Offshore Hubs, that is, hubs for offshore activities, which allow integrated exploration of

maritime resources, through more sustainable economic exploration routes with a lower carbon footprint. The methodology adopted was bibliographical research, obtaining direct and indirect data from official bodies, in addition to research in scientific literature, using the deductive method. The results point to the use of VLFS in the pre-salt polygon due to the abundant potential supply of energy, in the form of combustible gases, which, to date, have proven difficult to be transported to the Brazilian coast or for export. These large floating structures can then be designed for future integrated offshore natural gas processing, CO2 conversion, LNG liquefaction or offshore electricity generation projects, as well as for offshore fuel storage and as a CO2 injection hub in offshore CCUS systems. To date, they have proven difficult to transport to the Brazilian coast or for export. These large floating structures can then be designed for future integrated offshore natural gas processing, CO2 conversion, LNG liquefaction or offshore electricity generation projects, as well as for offshore fuel storage and as a CO2 injection hub in offshore CCUS systems. To date, they have proven difficult to transport to the Brazilian coast or for export. These large floating structures can then be designed for future integrated offshore natural gas processing, CO2 conversion, LNG liquefaction or offshore electricity generation projects, as well as for offshore fuel storage and as a CO2 injection hub in offshore CCUS systems.

Keywords: Floating Structures; oil and gas; energy; VLFS, greener offshore hubs.

Introduction and Objectives: Very Large Floating Structures (VLFS) are floating parcels of land constructed artificially by man in the sea. These structures are similar to giant plates floating on the sea surface, which are classified as semi-submersible or floating (SH Lin and CM Wang, 2015). Semi-submersible floating structures are elevated above sea level using columns or structural ballast elements to minimize the effects of waves while maintaining a constant buoyancy force. Thus, they can reduce wave-induced movements and are therefore suitably deployed in high seas with large waves. Floating oil drilling platforms used for oil and gas drilling and production are typical examples of semi-submersible VLFSs (SH Lin and CM Wang, 2015; CM Wang; ZY Tay, 2011). In contrast, floating-type structures sit at sea level like a giant plate floating on water. These structures are suitable for use in calm waters only, generally within a cove or lagoon and close to shore. Large floating structures were called Mega-Floats by Japanese engineers (SH Lin and CM Wang, 2015; CM Wang; ZY Tay, 2011). If in the past, in addition to maritime transport, the offshore business was dominated by the oil industry, in more recent years companies venturing into the seas have become more diversified. Very large floating structures (VLFS) have attracted the attention of architects, urban planners and engineers because they provide an interesting and environmentally friendly solution for creating land from the sea. The applications of VLFS such as floating piers, floating hotels, floating fuel storage facilities, floating stadiums, floating bridges, floating airports and even floating cities have triggered extensive research studies over the past two decades (CM Wang; ZY Tay, 2011). In Brazil, given that natural gas production in 2019 was on the order of 139 million m^3/day, with an increasing trend towards 2029, reaching levels of around 253 million

m³/day, the installation of VLFS in areas Pre-salt oil emerges as an alternative for monetizing natural gas reserves at the production site since the flow of exploited gas is complex and expensive due to the distance from the location (EPE, 2020). In this sense, the objective will be to explore the challenges for implementing VLFS projects in Brazil, taking into account technical-economic feasibility, construction aspects and legal and technological challenges for construction and installation. The various opportunities to be explored in Brazil with VLFS projects will also be the subject of this study, such as integrated offshore natural gas processing projects, CO2 conversion, liquefactionTheLNG or generationTheoffshore electricity, offshore fuel storage and injection hubTheCO2 in offshore CCUS systems.

Methodology: The methodology adopted was bibliographical research, obtaining direct and indirect data from official bodies, in addition to research in scientific literature, using the deductive method. In this way, bibliographical reviews will be carried out focusing on the use of VLFS structures to compose HUBS and/or offshore production clusters, on initial economic modeling to study the echnical-economic feasibility of VLSF structures and on constructive aspects and technological challenges for construction and installation of VLSF structures. The study also consists of the description of international cases of HUBS and/or clusters, which will later be analysed and modelled under an economic bias with application in Brazil. The technological, constructive and logistical challenges of VLSF will be highlighted and application opportunities in the country will be analysed.

Preliminary results: Preliminary studies showed important opportunities for implementation in Brazil. There is a floating one that combines offshore wind, solar and hydrogen energy solutions, including a storage island, along the lines of the conceptual framework project proposed by Spain's ACCIONA. Due to the country's port conditions and limitations, as well as efforts to develop cabotage activities, the Offshore Port concept also proved to be viable for the country, with important benefits for Offshore Hubs, such as projects developed by Bechtel. Applications of VLFS were also identified in the context of scientific research, defense, energy generation and installation of industrial units or floating electrical generation. The study also identified important development opportunities in the academic area, especially in Brazil. Through a survey carried out through the Scopus database (in June 2022), which results in only 559 documents published since 1978, although there has been a recent increase in publications on the topic. In Brazil, only one publication related to the topic was identified, in which a free vibration analysis of thick square plates was carried out using the boundary element method (BEM). Their results help to analyse hydroelastic issues of VLFS, which are usually modelled as free-edge plates. Most publications on Very Large Floating Structures are concentrated in Asian countries, with emphasis on Japan, China and Singapore, which alone constitute almost three quarters of the total documents.

Preliminary conclusions: Basic conceptual aspects must be studied, including, among others,

technological mapping of existing and/or under design installations; characterization of technologies applicable to the deep marine environment; logistical aspects, with the possibilities of energy supply and other facilities for these infrastructures, as well as logistical difficulties for their construction and installation. Furthermore, analyse some essential construction elements, including a discussion about the materials needed to execute these installations, as well as identify technological challenges of these solutions that still deserve additional research. Preliminary models will be developed to enable assessments of the economic and financial viability of these projects to begin. For these analyses, the models will focus on the reality of offshore O&G production in Brazil, as suggested above. In fact, it is understood that the creation of a long-term system, through the construction of VLFS, opens up technological alternatives for using natural gas available in remote offshore fields, with high concentrations of gas, such as those in the pre-salt region, since gas becomes an abundant and viable source of energy, available locally, to sustain the proposed operations for the VLFS. Considered a disruptive approach, this work is also dedicated to raising possible gaps in the normative and regulatory fields, both within the Brazilian legal environment and in the experiences of international law. Based on legal and normative mappings, it is possible to propose instruments that need to be designed in Brazil so that the country can house VLFS-type structures in the future.

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Abstract Title: Strategic route for CO2 transportation in the state of Rio de Janeiro

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Abstract: The present study seeks to contribute to the discussion of the importance of defining strategic routes for CO2 transport in the Brazilian carbon capture and storage (CCS) scenario. To this end, a case study was developed to define a CO2 transport route, evaluating the Brazilian oil and gas infrastructure and its compatibility and availability for use in the CCS system. According to the 2019 Indicative Plan for Processing and Flow of Natural Gas (PIPE), in Brazil the national net production of natural gas should increase from 59 million m³/day in 2018 to 147 million m³/day in 2030. Consequently, the installation of new natural gas processing and transportation infrastructures or the expansion of existing ones will be imperative to enable the monetization of natural gas production projected for the coming years. Based on this information, it is unfeasible to design the transport of CO2 through existing natural gas

pipelines, since the existing structure already operates at full capacity and, therefore, urgent expansions are anticipated. Thus, the case study addressed will be dedicated to the establishment of a strategic route for the transport of CO2 resulting from the production of nitrogen fertilizers that uses natural gas as a raw material. It was also defined that a CO2 capture hub would be installed from sources other than the fertilizer plant. The definition of the location of the capture hub considered the CO2 emissions inventory of the State of Rio de Janeiro and, based on it, the Duque de Caxias region was defined for the installation of the capture hub, as it has an extensive network of natural gas and, in addition, it is an industrial region with the highest annual CO2 emissions, reaching approximately 24 million tons of CO2EQ per year. In this scenario, the captured CO2 will be stored in a depleted offshore oil and gas production field. Furthermore, with the scenario analyzed, it was concluded that it is necessary to install a new gas pipeline to transport CO2, covering a strategic route of approximately 180 km on land and 210 km on the high seas. The onshore gas pipeline begins in the region of Duque de Caxias, RJ, and ends near Tecab, in Macaé, RJ, taking advantage of the existing Dasduc III gas pipeline corridor, which also has terminations in the regions of Duque de Caxias and Tecab (Macaé). The construction of a new gas pipeline within an existing corridor can result in a cost reduction in the project. In the case of the offshore route, it originates in the Macaé region and ends in the Roncador field, in the Campos basin, whose CO2 storage capacity is approximately 265 MTCO2. If 16 additional fields are considered in the Campos basin, the CO2 storage capacity can reach around 950 MTCO2. It is worth mentioning that the construction of the offshore route can take advantage of the mobilization and infrastructure of upcoming offshore oil and gas exploration projects in the pre-salt region.

Keywords: Transport CO2, Route Strategic, Brazil CCS.

Introduction and Objectives: Although there is much debate about the dangers of excessive fertilizer use on a global scale and the environmental pollution it generates, it is known that fertilizers have played an essential role in feeding the world's growing population. Currently, 81% of the world's ammonia production is destined for the manufacture of nitrogen fertilizers, whose main raw material is ammonia, which uses hydrogen produced from the catalytic reforming of natural gas, resulting in the production of hydrogen and CO2. In 2018, global ammonia production was around 176 Mt, responsible for around 1.8% of global carbon dioxide emissions. Brazil uses, directly or indirectly, around 4% of the world's ammonia production in the form of fertilizers. Of this, around 80% is imported.

In view of this scenario and the need to monetize pre-salt natural gas, the aim of this work is to study the location for the installation of a nitrogen fertilizer production plant and a strategicroute for transporting the CO2 resulting from the manufacture of fertilizer by pipeline to the storage site in the Campos Basin, i.e. the plant will use blue hydrogen to produce ammonia.

Methodology: The study methodology was the elaboration of a case study from the information obtained in the bibliographic review. In the bibliographic review process, institutional reports and scientific documents were consulted. In this document, information on

production and consumption of fertilizers and ammonia; production, consumption and logistics of natural gas in Brazil and finally information about CO2 emissions in the state of Rio de Janeiro. were researched.

Preliminary results: The proposed strategic route for transporting CO2 captured at the fertilizer plant and region will be approximately 180 km of onshore pipeline and 210 km of offshore pipeline. A shorter offshore route could be achieved, resulting mainly in lower implementation costs, if it departed from the Porto do Açu region, in the municipality of São João da Barra / RJ, instead of the Macaé region. This route would have a length of approximately 130 km until reaching the Roncador field, however, when studying CO2 transport, the entire CO2 capture and storage chain must be evaluated. The offshore route that departs from the Macaé region (beginning) and heads towards the central region of the Campos Basin will, in the future, enable interconnections to be made, thus allowing other depleted reservoirs in this basin to be connected and used for CO2 storage. Studies show that CO2 storage capacity can increase from approximately 265 MtCO2 to 950 MtCO2, if another 16 reservoirs in the Campos Basin are added. This also applies to the possible depleted reservoirs

in the Santos Basin, since it is located on the Brazilian coast just below the Campos Basin. As for the onshore route, it allows capturing CO2 from the metropolitan region of Rio de Janeiro and, in the future, adding it to the northern region of Rio de Janeiro. When thinking about a route from the Port of Açu region, the ability to establish a CO2 capture hub in the main industrial region of the state of Rio de Janeiro is lost.

Preliminary conclusions: However, it is necessary to plan strategic routes for transporting CO2 to the storage point. The study shows that advance planning can help reduce costs and predict the best location for the transport hub and injection of captured CO2.

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RCGI InnovaPower Programme - Project08

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Abstract Title: A survey of subsea equipment for offshore transmission systems

Authors' Names & Affiliation Institutions of all authors (in order for publication): Isabela Corrêa Hillal (Poli-USP), Luís Felipe Normandia Lourenço (IEE-USP), Maurício Salles (Poli-USP)

Abstract: This research project aims to evaluate the integration of offshore wind farms into the Brazilian electrical grid, considering a variety of transmission technologies for future developments along the coast. The overall scope of the project seeks to systematically expand offshore transmission systems, contributing to energy transition and decarbonization, both in Brazil and globally. This particular work focuses on creating a comprehensive report addressing crucial underwater equipment for the execution of activities related to this project. This will include a detailed analysis of their applications, functionalities, and the technologies employed. The primary emphasis will be on verifying the technological limits of these underwater equipment and tracking their evolution over the years, from their initial applications to the current scenario.

Keywords: Offshore Transmission, Offshore Wind Power, Subsea Power Cables, Subsea equipment.

Introduction and Objectives: Offshore transmission systems serve the purpose of transporting electricity generated in renewable energy installations located at sea, such as offshore wind, to the coast or other consumption points. These systems comprise various components and technologies essential to ensure the effective and reliable transmission of energy generated at sea.

Offshore substations, located near offshore energy parks, are responsible for collecting, transforming, and distributing the electricity generated by wind turbines or solar panels. They are equipped with transformers and other control devices to adjust electrical voltage before transmission. Moreover, submarine cables play a crucial role in transmitting the electricity generated offshore to the coast or other consumption points. These cables are designed to withstand adverse maritime conditions such as strong currents, waves, temperature changes, and pressure fluctuations.

Two common types of cables are currently in use: MI cables, which have solid insulation composed of resin impregnated with insulating materials, filling the spaces between and around the conductors completely. These cables are known for their resistance to high temperatures, excellent mechanical protection against external damage, and extended lifespan due to moisture and contaminant prevention. In addition to MI cables, XLPE cables also play a significant role in the market. XLPE refers to the insulating material used, which is cross-linked polyethylene. This insulation is known for its high dielectric strength, allowing for the use of higher voltages in cables, making transmissions more efficient. XLPE cables also withstand heat well, making them suitable for high-temperature environments, and have low dielectric loss, reducing energy losses during electrical transmission, making them energy-efficient. Several factors can

influence the determination of the voltage and power that each cable will be able to transport. Cable length is one of them, as the longer the distance a submarine cable needs to traverse, the higher the resistance along the cable. This can result in power losses and voltage drop along the cable. To compensate for these losses, reinforcement or amplification equipment may be required along the cable to maintain adequate power and voltage levels. The primary objective of this study is to conduct a comprehensive synthesis and a meticulous analysis of the factors affecting the determination of stresses and power levels in submarine cables used in offshore HVDC transmission. The intention is to comprehend the influence of these factors and, thus, gain a clear insight into the technological constraints of the components available in the current market as they have evolved over the years. Initially, the factors to be taken into consideration include the solution type, cable type, location, commissioning year, length, and water depth.

Methodology: With the purpose of conducting a comprehensive analysis of HVDC cables used in offshore transmission, it is planned to include various manufacturers of this component in the research. For each manufacturer, a table will be developed containing essential information about their projects. The data to be addressed include the name of each project, as well as information such as solution type, cable type, location, voltage, power, length, and water depth. Such information will be obtained through official disclosures from technology manufacturers, as well as published studies that identify the names of the analysed projects. By compiling this data, it will be possible to create graphs that establish relationships between the various parameters that can influence the technological limits of the cables, along with their respective voltages, powers, and commissioning years. Based on this information, it will be possible to draw conclusions about the evolution of this technology over the years and formulate hypotheses about the technologies available in the current context. It is essential to emphasize that the more data and details are meticulously mapped, the more accurate the results obtained will be.

Preliminary results: This Is a recently started scientific initiation project. The expectation is that the results obtained will provide a comprehensive analysis of the modifications that each parameter, as listed in the table, exerts on voltage and power variations. The primary objective of this project is to conduct meticulous research to assess the current state of offshore equipment relevant in today's scenario, taking into consideration its evolution over the years. The project aims to integrate technological aspects into a single report, which will serve as a comprehensive synthesis of this landscape. So far, no concrete results have been obtained as only one company, NKT, has been analysed. To complete the table for this company, some data related to the length and depth of some of the 28 offshore HVDC transmission projects under analysis in this work are still missing. The lack of information is due to the difficulty in finding reliable sources that provide these specific values for some of the projects. However, concerning one of the columns already filled with data disclosed by NKT on its official website, which pertains to the solution type, interesting information has been observed that corroborates the statements made in the introduction regarding this parameter. Specifically, it has been noted that of the 28 analysed projects, with 25% related to offshore wind energy, 14.3% to Power From Shore, and 60.7% to

Interconnector and power transmission, all projects with the highest voltages (350kV-525kV) belong to the Interconnector and power transmission type, confirming what has been discussed in the previous sections. Furthermore, the 4 projects related to Power From Shore are concentrated in the two lowest possible voltages, 80kV and 90kV.

Preliminary conclusions: The purpose of this scientific research project is to establish the technological limits of essential equipment for submarine transmission, which play a crucial role in integrating offshore wind farms along the Brazilian coast. Given that operating in such rigorous and challenging environments requires the development of highly specialized equipment, this project aims to provide a valuable resource for those involved in offshore wind energy exploration. It seeks to compile information and data about this equipment in a single report. The resulting dataset will be a comprehensive synthesis of the current market landscape, highlighting the uniqueness of each project, taking into consideration the natural characteristics of their locations, and the specific demands of each undertaking.

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Abstract Title: Simulation of Power Inverters and Controls in Grid-Connected Wind Systems
Authors' Names & Affiliation Institutions of all authors: Helena Marques Almeida Silva - Universidade de São Paulo (USP), Renato Machado Monaro - Universidade de São Paulo (USP)

Abstract: Wind generation has increased its relevance in the Brazilian electrical matrix.

However, the penetration of this renewable source into the electrical system requires the connection of inverters at the interface between the generator and the grid. Such equipment interacts with the capacitive elements of substations and transmission lines, which can cause resonances. As this is a recent issue, there are no robust techniques in the industry to detect and mitigate the occurrence of these events. In this context, the objective of the project is to implement models of inverters and their most common controls connected to transmission systems, using the Simulink software. Thus, we hope to better understand the impact of inverters on the electrical system.

Keywords: Wind energy, power inverters, control, resonances, Simulink

Introduction and Objectives: Among the UN's sustainable development goals for Brazil is clean and affordable energy. To achieve this goal, it is necessary to intensify investments in renewable energy sources, increasing their participation in the country's electrical matrix. Currently, the wind source has 26 GW of installed capacity in commercial operation, according to ABEEólica. However, despite its growth potential, the insertion of wind turbines into the electricity grid contains an issue. In order to optimize the power generated, it is desirable that wind turbines operate at variable speed. Power inverters are used for this. The interaction between the inverters and the capacitive elements of the network can generate resonances in harmonic frequency ranges (above 60Hz), for shunt capacitors, and in subsynchronous frequencies (below 60Hz), for series capacitors. Furthermore, inverters behave like a negative resistance in the network, weakening the damping of resonances, which leads to the flow of high electrical currents that damage equipment and shorten its lifespan. In this regard, the project aims to build and simulate inverter models used in the wind energy scenario, in addition to its more usual controls, which dictate the injection of active and reactive power, using Simulink. In this way, we expect to better understand the impact of these equipment on the network.

Methodology: The methodology of this project consists of a literature review, implementation and validation. Two months of a literature review are planned on power inverter models (switched and average) and control techniques. Next, each model and its most common controls will be implemented in the Simulink software, which is expected to take three months for each model. Finally, the simulation results will be validated with models present in the literature, a two-month step.

Preliminary results: Since the project began in August, there are no simulation results to be presented so far. The literature review learning stands out, when some principles of wind generation were studied, such as the importance of control for maximum power production (MPPT), the main models of generators used, voltage-oriented control, PI (proportional-integral) and PR (proportional-resonant) controls.

Preliminary conclusions: Considering that the current stage is a literature review, there are still no conclusions to be presented.

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We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Methods for analysis and mitigation of resonances in DER-rich distribution systems

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Abstract: Modern electrical energy distribution systems are experiencing significant changes, especially with the rapidly increasing penetration of distributed energy resources (DERs), such as photovoltaic and wind generators, electrical vehicles, and energy storage systems. These devices use power electronic-based technologies, which may present negative resistance characteristics at specific frequencies. Therefore, these power electronic-based DERs have the potential to decrease resonance damping in the electrical system and, consequently, damage circuit equipment and customer loads (customer processes). This can create significant financial losses not only to the distribution utility, but also to the end customer. As the high penetration of DERs in distribution systems is a relatively recent trend, it remains unclear which are the main characteristics and most critical scenarios of these resonances. In addition, there are no well-established methods to anticipate the risk of these problematic resonances and mitigate them. In this context, the goal of this project is to provide a detailed characterization of these resonances in DER rich distribution systems and develop methods to predict the risk of occurrence of these resonances and mitigate this risk, avoiding costly damages to circuit equipment. The focus is on the development of systematic methods that can speed-up the decision-making process of engineers in terms of which actions should be undertaken to avoid or eliminate resonances, either during planning or operation of DER-rich distribution systems. The results of this project will be used not only to reduce the risks and costs associated with technical losses and device damages, unplanned disconnection of customer processes, equipment lifetime reduction, and number of man-hours needed to manage these resonances.

The results of this project can also be used to support the improvement of national regulations for DER integration into the distribution systems.

Keywords: resonance; distributed energy resources; DER; capacitor; mitigation; prediction; power electronic converters.

Introduction and Objectives: Recently, electric power distribution systems have migrated from a passive, non-supervised structure with low level of automation to an active, supervised structure with high level of automation due to the introduction of DERs and new automatic control devices. The most common DERs include wind turbines, electric vehicles chargers, energy storage systems and, primarily, photovoltaic generators. In Brazil, it is estimated that PV generation will account for over 97% of the distributed generation capacity installed over the next decade. A common characteristic of these DERs is that they have a power electronic converter as their interface with the grid.

In terms of new utility devices installed in the system, in the context of this work, it is important to highlight automatically operated capacitor banks, which can be installed at Medium Voltage (MV) grids, as usual, or even be installed dispersedly over the system at the Low Voltage (LV) grids, and a more frequent installation of switched series capacitor banks to supply loads or distributed generation at locations far from the substation. The increased presence of shunt and series capacitors combined with the increased presence of power electronic-based DERs has the potential to increase the amount and severity of resonances in the circuit. The reason is that the power electronic converters used in DERs (mainly the voltage source converters) can have a negative resistance characteristic at specific frequencies. If a negative equivalent resistance matches a resonance frequency in the circuit, the resulting effect is that resonance damping will decrease (creating weakly damped resonances) and potentially become negative (creating unstable resonances), which can damage circuit equipment and create significant financial losses to the distribution utility and to the customers. This effect can happen both at LV systems, where shunt capacitors are being installed, and at MV systems, where shunt and series capacitors are installed. One challenge with this scenario is that distribution utility engineers are not traditionally concerned with weakly damped resonances and instabilities and tend to address them on a case-by-case basis, which are normally based on numerous detailed electromagnetic transient or frequency-domain simulations. However, with the increased penetration of DERs, such events are bound to become more frequent. Hence, it is essential to investigate and develop new approaches to systematically manage the risk of these events without the need to run time-consuming computer simulations. The main objective of this research is to investigate the characteristics of resonances in power distribution systems with high penetration of DERs and develop practical methods for managing (anticipating and mitigating) the risk of these events.

Methodology: Two main types of resonances will be investigated: resonances on LV distribution systems and resonances on MV distribution systems. More specifically, LV

systems are smaller, and the predominant inductance is from the distribution transformer (line inductances can be neglected in most cases), whereas MV systems are larger, and the line inductance is significant. Adverse events on LV systems affect a few tens of customers, whereas an equivalent event on MV systems affects thousands of customers. DERs installed in LV systems are mostly single-phase devices (although some three-phase devices may also exist), whereas DERs installed in MV systems are three-phase devices. These different characteristics highlight that the behavior of resonances on LV systems is expected to be different (different root causes, different participation factors of the DERs, different mitigation approaches etc.) from the behavior of resonances on MV systems. For each type of resonance, the following specific objectives can be outlined: - Characterization: investigate and identify the main causes of the event and the critical scenarios where it can be initiated, which consists in identifying the parameters of the DER and of the power system with highest impact on the risk of resonance;

- Detection of the risk of occurrence: develop methodologies for the expedited and systematic identification of the risk of resonance in distribution systems, based on the characteristics (topological and operational) of the circuit;

- Mitigation of the risk of occurrence: develop methodologies to mitigate the risk of resonance in a distribution circuit (avoiding the onset of an event), or to mitigate already ongoing resonances; and - Power-Hardware In the Loop Simulations to evaluate the methods developed. The knowledge obtained during this research and the methodologies developed will create the technical basis to support potential improvements on the national regulation about the integration of DERs.

Preliminary results: As the project is in its early stages, there is no Preliminary results.
Preliminary conclusions: As the project is in its early stages, there is no Preliminary conclusions.

0711 - GHG4 (TV4)

Chairs: Emílio Carlos Nelli Silva – Luis Fernando Sá

Anderson Soares da Costa Azevêdo
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Abstract Title: On the topology optimization of CO2 labyrinth seal design considering forward and backward incompressible laminar fluid flow regime

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Abstract: To address the concern of carbon dioxide (CO2) emissions, the optimization of labyrinth seals presents a paradigm-shifting solution. These seals are meticulously engineered to minimize gas leakage from compressors stages until the atmosphere, thereby facilitating the development of highly efficient seal designs. Labyrinth seals can be seen as a type of fluid diode commonly employed by the metallurgic industry in pneumatic machines. Traditional literature usually adopts parametric and shape optimization as the main tools to improve the design of these fluidic devices. Therefore, there is plenty of room for fill the scientific gap of topology optimization on seal applications. This work discusses the use of topology optimization in the synthesis of labyrinth fluid diodes. The labyrinth fluid flow path should be designed to be favored in one direction (forward) while unfavored in the opposite direction (backward). This optimization task poses a challenging problem for topology design. In this work, we employ the TOBS (Topology Optimization of Binary Structures) method to solve a 2D prismatic and axisymmetric seal problem. We maximize the diodicity by minimizing the forward energy dissipation while maximizing the backward vorticity subjected to a fluid volume constraint. The steady state Navier-Stokes equations govern the 2D flow with the standard Darcy term used for topology optimization. The governing equations are solved via the Finite Element Method considering prismatic and axisymmetric configuration, and the optimization problem is solved by the TOBS method. The TOBS is a gradient based method that produces a sequence of linearly approximated problems and solves them via integer linear programming. The numerical example shall elucidate how solid permeability influences topology evolution. We assumed real CO2 gas properties and realistic dimensions for the seal. Finally, our method predicted that the porous material model favors radial interlocking teeth labyrinth in the seal. Therefore, TOBS has shown to be a potential method for seal design.

Keywords: Discrete design variables, integer linear programming, diodicity.

Introduction and Objectives: Traditional fluid diodes topology optimization is done

considering a continuation procedure to reduce the fluid infiltration issue on the regions emulated as solid. The currently available methods produce large quantities of floating solid islands instead of complex interlaced arrangements along the designed chamber which are not viable for labyrinth fluid diode applications, such as in pneumatic machines. Thus, this work has two main goals to fill this scientific gap. First, an alternative weighted multi-objective logarithmic expression that induces a labyrinth fluid path by combining fluid flow energy dissipation and vorticity magnitude is proposed. Second, it is demonstrated that the proposed function can design labyrinths for maximizing diodicity similar to traditional literature objective function that uses only energy dissipation terms.

Methodology: Generalized fluid flow governing equations including the Darcy term are solved with an external Finite Element Analysis package, a built-in automatic differentiation

module is used to perform the sensitivities computation, and the design variables are updated via the TOBS method through Sequential Integer Linear Programming. A regular mesh of quadrilateral elements is adopted for both flow directions assuming respectively quadratic and linear basis for velocity and pressure fields. This procedure was implemented in COMSOL Multiphysics LiveLink with MATLAB. A continuation procedure combining two convergence criteria (objective function and material distribution change) is used to pursue robust solutions.

Preliminary results: - Bidimensional axisymmetric geometry poses a harder optimization problem than the prismatic case and is sensible to shaft diameter values
- Improve the diodicity expressed in terms of energy dissipation and vorticity can increase pressure drop of seal devices
- The topologies obtained are suitable for prototype manufacturing via 3D printing

Preliminary conclusions: - Bidimensional axisymmetric and prismatic geometry present distinct evolution behavior - The interlocking teeth direction between rotor and stator is influenced by solid permeability - The dependency of a local minima to the material model penalization can be reduced by using two convergence criteria into a continuation approach
- The proposed strategy can help to reduce the gas escape on seal devices and then lead to lower fuel consumption and emission in power generation and transportation sectors

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André Dantas Freire
University of Sao Paulo

Abstract Title: numerical prediction of erosion in labyrinth seals: A Lifespan approach

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Abstract: Labyrinth seals (LS) are commonly employed to mitigate leakage but are susceptible to erosive wear resulting from fine particulate matter in turbomachinery systems. This study aims to simulate erosion rates in rotor labyrinth seals utilizing Finnie's model to assess the erosive impact on leakage. Variations in alloy properties, achieved through additive manufacturing, including density (ρ) (4252, 4297, and 4341 kg/m³) and surface hardness (H) (3.0, 3.5, and 4.0 GPa, corresponding to 313.4, 365.8, and 418 HV/10), were considered. SiC spherical particles (Dp) were introduced to induce erosion during simulations (100µm, 150µm, and 200µm). The findings reveal that hardness and density variations did not exert a significant influence. Finnie's model exhibits a superior predictive capability when particles are entrained

and impact the wall at shallow angles (low Re). The tooth lifespan estimation chart delineates the maximum expected service life of the initial labyrinth seal tooth, demonstrating a wide range of resistance to erosive wear, from as little as one day to as long as twenty years.

Keywords: Labyrinth Seal; Erosion Wear; Lifespan.

Introduction and Objectives: Labyrinth seals (LS) are frequently employed to reduce leakage but are prone to erosion from fine particles in turbomachinery systems. This research endeavors to simulate erosion rates in rotor labyrinth seals by applying Finnie's model, with the objective of quantifying erosion's influence on leakage [1].
Methodology: The erosion wear in the labyrinth seal (ten teeth) made of Ti-6Al-4V alloy is predicted using the Finnie erosion model, which considers particle velocity, diameter, and impact angle [2]. The alloy, obtained by additive manufacturing, density (ρ) (4252, 4297 and 4341 kg/m³) and surface hardness (H) (3.0, 3.5 and 4.0 GPa – corresponding to 313.4, 365.8 and 418HV/10) were varied considering [3]. The fluid flow within the LS on a rotor is modeled using the incompressible Navier-Stokes equations using the software COMSOL. The turbulent flow of CO2 is simulated using the Reynolds-averaged Navier-Stokes (RANS) equations. The dynamic viscosity of 1.47e-5 [Pa s] and density of 1.84 [kg/m³] of CO2 were used. Reynolds numbers (Re) of 200 and 2000 were evaluated to represent low and high inlet velocities. The rotational speed was 1018 rpm (rotor rotation). SiC spheric particles (Dp) were added to cause erosion during simulation (100µm, 150µm, and 200µm), which can be found in oil and gas transportation [4]. A function was used that relates the geometric conditions and tooth material, erosion wear time, and erosion wear rate to perform functional lifespan calculations in the tooth.

Preliminary results: The longevity of a labyrinth seal tooth is depicted under various wear conditions, characterized by different particle velocities and diameters. Elevated particle velocities associated with higher Reynolds numbers resulted in erosive wear, causing a single tooth measuring 1 millimeter to endure only one day of service life. At intermediate Reynolds numbers (Re 2000), the tooth exhibited a wear pattern culminating in an approximate operational lifespan of 5 years. Conversely, under lower Reynolds number conditions (Re 200), the same labyrinth seal tooth demonstrated remarkable durability, with a service life exceeding 20 years. Figure 2 shows the main factors that represent the significant levels: Re and Dp. The other factors (the H and Density) do not significantly affect erosion ($p > 0.05$). In Table 1, an overview of the influential factor levels in the investigation of erosion wear within rotor labyrinth seals is presented. The parameter 'Re' is found to contribute 22.66% to the variability at both the 200 and 2000 levels. Meanwhile, 'Dp' demonstrates a 3.42% influence on variability at levels 100, 150, and 200. Furthermore, the interaction between 'Re' and 'Dp' is responsible for a 2.60% contribution to variability across all levels, with due consideration for associated measurement errors.

Preliminary conclusions: Hardness and density have not had a significant effect. Finnie's model shows the best results for small Dp and low Re. Therefore, Prudent management of

particle size assumes paramount significance within the context of turbines and compressors, given its potential to markedly amplify the erosion rates experienced by labyrinth seal teeth. Such accelerated erosion wear invariably leads to a substantial reduction in system efficiency and power generation output. Moreover, the repercussions of premature maintenance procedures in a turbine can result in a substantial escalation of operational expenses.

Ben-hur Martins Portella
University of São Paulo

Abstract Title: Numerical modeling of sources and sinks of greenhouse gases in the Amazon during the CAFE-Brazil experiment

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Abstract: The Amazon forest plays an important role in the terrestrial carbon balance, influencing the energy balance and climate on a regional and global scale. The Amazon region acts as a carbon sink, through the photosynthesis process, and, at the same time, acts as a carbon source, through emissions from fires and flooded areas. Research indicates that the fluxes of greenhouse gases (GHG) carbon dioxide (CO2) and methane (CH4) are spatially heterogeneous in the Amazon. Variations in the magnitude of emissions are associated with changes in meteorological variables such as temperature and precipitation, as well as changes in land use and fires. It is essential to characterize the sources and sinks of GHG in the Amazon in their natural state, in order to understand the possible dynamic adaptations of the ecosystem in the face of climate change. This project aims to estimate sources and
sinks of CO2 and CH4 in the western Amazon during the rainy season, using an inversion strategy based on computational simulations and in situ observations. The regional model WRF-GHG (Weather Research and Forecasting, coupled to the greenhouse gas module) will be used to simulate the distribution of GHG concentrations in the western Amazon, where

almost pristine conditions predominate during the rainy season. The simulations will be contrasted with observations collected during two intensive experiments (CAFE-Brazil and FLOAT). With this, it is expected to identify the relative contribution of different types of biogenic GHG sources and sinks in this region of preserved tropical forest, in addition to identifying possible areas that act as emission hotspots.

Keywords: Amazon; Modelling; Greenhouse Gases; CAFE-Brazil; FLOAT.

Introduction and Objectives: As the largest tropical forest on the planet, the Amazon plays

a relevant role in the climate system. Among the environmental services provided by the forest, we can highlight the storage of carbon in the form of biomass and in the soil, estimated at around 150 Pg C. In general, the forest acts as a sink for the greenhouse gas (GHG) carbon dioxide (CO2), with a net removal of about 0.4 ± 0.1 Pg C/year from the atmosphere, considering the processes of photosynthesis and respiration. However, long-term observations indicate that this removal rate can decrease or even be reversed in dry years, revealing the existing coupling between biogeochemical cycles and the hydrological cycle. In recent decades, a consistent increase has been observed in the duration of the dry season in the Amazon (Marengo et al., 2018), increasing the forest's vulnerability to climate change with impacts on the carbon balance. In addition to CO2, another GHG of great relevance is methane (CH4). Despite not being as abundant in the atmosphere as CO2, CH4 has a Global Warming Potential (GWP) 28 times greater on a 100-year time scale, contributing about a quarter of the effective radiative forcing of GHGs. CH4 is mainly produced by the anaerobic decomposition of organic matter, through cooperation between different microbial cultures. Wetlands constitute the main natural source of CH4 to the atmosphere, accounting for 32% of global emissions. In particular, emissions from flooded areas in the tropical region constitute the greatest source of uncertainty for the global balance, due to the scarcity of in situ observations and the typical variability of emissions, related to the complexity of production, transport and consumption of methane until it reaches the atmosphere. The land use change sector contributes to anthropogenic CH4 emissions through fires and the conversion of forest areas into agricultural areas. Observational studies indicate that the Amazon contributes around 8% of global CH4 emissions, with 73% of emissions coming from flooded areas, 17% from fires, and 10% from other anthropogenic sources associated mainly with enteric fermentation in ruminants. Hydroelectric reservoirs in the Amazon also emit CH4, mainly through degassing in turbines and downstream. The general objective of this project is to estimate sources and sinks of CO2 and CH4 in the western Amazon during the rainy season, combining computational simulations with a regional atmospheric transport model and in situ observations. As specific objectives, we can list: Identify the relative contribution of different types of biogenic sources and sinks of CO2 and CH4; Characterize the spatial distribution of GHG concentrations in the western Amazon, identifying strong emitting areas (hotspots); Simulate CO2 and CH4 emissions under different climate and deforestation scenarios.

Methodology:

The project is organized in the following steps:

1. Bibliographic review on the WRF model and greenhouse gases in the Amazon; 2. Compilation of data from the FLOAT-CAFE experiment;

3. Definition of the simulation configuration, depending on the spatial distribution of the collected observational data;

4. Pre-processing of input meteorological fields;

5. Preparation of initial and boundary conditions for GHG concentration and emission; 6. Comparison between the results of the first simulations with observational precipitation and radiosonde data;
7. Adjustment of GHG emissions based on comparison with observational data; 8. Analysis of computer simulations;

Preliminary results: A bibliographical review of previous works that used the WRF, with different components, for analyzes aimed at the Amazon or the tropical region was carried out. Furthermore, the various options for physical parameters and model configurations were studied, in order to identify the best configurations considering the local climate and vegetation. Finally, the first reproductions of the domains used, as well as the initial simulation of the model, were made by the student during the course of their learning.

Preliminary conclusions: Since this is an initial period of understanding the model to be used, the student made an effort to record their learning and instructions, thus creating an installation and preparation guide for both the pre-processing system and the model itself. Additionally, a document was prepared summarizing the main physical parameters applicable to the model and relevant to the scope of the research.

Carlos Eduardo Lino
University of São Paulo (USP)

Abstract Title: Topology Optimization Method Applied to the Design of Radial Compressors Considering Turbulent Real Gas Flow Through Fluid-Structure Interaction and Mechanical Fatigue Analysis

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Abstract: Fossil fuels, including coal, oil, and natural gas, play a critical role in energy generation due to their high energy output per unit of mass. Within the oil and gas industry, radial compressors play a vital role in processing and transporting gases. However, their environmental impact is significant, primarily due to the release of greenhouse gases (GHGs) and other pollutants. Particular concern are carbon dioxide (CO2) and methane (CH4), given their substantial contribution to climate change. This study aims to develop a systematic topology optimization method for designing radial compressor rotors, specifically targeting the use of real CO2 gas or a CO2-CH4 mixture. The proposed method simplifies the coupling

process between fluid and structure by emphasizing a strong interaction of degrees of freedom within both domains. Moreover, mechanical fatigue analysis utilizing the Paris law is applied until a pre-crack forms in the solid component. This study aims to integrate diverse objective functions to address fluid-structure interaction (FSI), encompassing fluid-related efficiency, pressure ratio, as well as structure-related stresses and vibrations. To achieve this, novel topological optimization formulations will be developed, incorporating the Coupled Moment Method for FSI (CMM-FSI).
The numerical implementation of this approach will leverage the FeniCS Topopt Foam software. The thermodynamic behavior of the CO2-CH4 mixture will be modeled using the Peng-Robinson equation of state. Additionally, problem sensitivities will be calculated using FeniCS and the IPOPT (Interior Point OPTimizer) library, implemented in Python through the FEniCS library and Finite Element Methods. The anticipated outcome of this research is the development of an effective methodology for optimizing the behavior of fully compressible and turbulent flows, thus contributing to compressor research and improvement while considering environmental impacts.

Keywords: Topology Optimization, Turbulent Flows, Fluid-Structure Interaction, Fatigue Analysis.

Introduction and Objectives: Fossil fuels (i.e. coal, oil and natural gas) are of great importance due to their ability to provide a significant amount of energy per unit of mass. Compressors are used for such a wide range of fluids, and complex models of real gas, turbulent compressible flow, are often needed to characterize fluid behavior. The research will be on Centrifugal (Radial) Compressors, to perform topological optimization to design impellers. Computational Fluid Dynamics (CFD) techniques play an important role as flow behavior can be predicted and studied accurately. To fully consider the best way to improve, the concept of optimal design must be understood, which is the best design among alternatives that meet a specified objective. Optimization is the mathematical process through which the set of conditions are obtained and produces the maximum or minimum value of a given function. A common way to classify optimization techniques is by dividing them into categories, with regard to the definition of design variables. Three main groups can be identified: parametric optimization, geometric shape optimization and topological optimization. Geometric deform optimization consists of changing the initial geometry, applying small displacements in the

domain. The geometry is parameterized and changed smoothly or any other method that to be able to describe a contour and sensitivities of a function, objective are calculated with respect to small variations in these descriptions of the geometry. In topology optimization, the objective of interest is minimized or maximized by distributing material within a design domain. Unlike other techniques, Topological Optimization allows opening and closing holes, resulting in greater design freedom with a wider range of possibilities.

1. Apply the topology optimization formulation to design radial compressors for operation with

real gas CO2 and/or CO2-CH4 mixture, address fluid-structure interaction (FSI), covering fluid-related efficiency, pressure ratio, as well as stresses and vibrations related to the structure. To this end, new topology optimization formulations will be developed, incorporating the Coupled Moment Method for FSI (CMM FSI).

2. Develop a topological optimization algorithm for compressible turbulent flows for real gas; implement discrete adjoint model of turbulent compressible rotating flows; with the discrete adjunct method to optimize the design and mechanical fatigue analysis using the Paris law is applied until a pre-crack form in the solid component;

3. Implementing an algorithm for resonant frequency restriction and analyzing the evidence of its impact on the impeller, will be implemented in Python using the FEniCS library with the IPOPT (Interior Point OPTimizer) library and OpenFOAM in C++; other libraries and optimization algorithms;

4. Develop topology optimization simulations to design rotors, aiming to maximize radial compressor efficiency;

Methodology: There are no preliminary results as the research is just beginning.

Preliminary results: There are no preliminary results as the research is just beginning.

Preliminary conclusions: There are no preliminary results as the research is just beginning.

Daniela Andrade Damasceno
University of São Paulo

Abstract Title: Computational Design of Nanostructures and Nanofluidic Systems by Coupling Molecular Simulations with Topology Optimization

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Escola Politécnica, University of São Paulo

Abstract: The rational design of nanostructures and nanofluidic systems with enhanced mechanical and physical properties is an emerging area. Nanofabrication and computational modelling advancements have provided powerful tools for inspecting and creating nanoscale systems. This study presents a new methodology called NanoTO for the computational design of nanostructures and nanofluidic systems by coupling molecular simulations with the Topology Optimization of Binary Structures (TOBS) method. By leveraging the strengths of both methods, we aim to unlock new possibilities and advance the development of highly efficient nanoscale devices. Our initial findings show that NanoTO can obtain optimised nanostructures with enhanced mechanical properties and optimised nanochannels to minimise pressure drop.

Keywords: nano-engineered structures, topology optimisation, mechanical properties, optimised nanochannel.

Introduction and Objectives: Pursuing optimal conditions and topologies is inherent in human nature and the natural world. Designing materials at the nanoscale enables the customisation of fundamental properties, serving as building blocks for advancing existing technologies and developing revolutionary devices with unique properties. These achievements stem from the precise manipulation of matter within a scale ranging from 1 to 100 nm, where materials' morphology, shape, and structure assume essential roles in shaping their fundamental properties. Researchers have turned to molecular dynamics (MD) simulations to understand molecular interactions better. These simulations track the movement of atoms, providing detailed insights into system behaviour and fundamental properties. However, it is crucial to go beyond traditional structures and explore new designs through optimisation strategies to unlock the full potential of nanoengineered systems. Topology optimisation (TO), a powerful computational method used in engineering, allows researchers to find an optimal distribution of materials within a given space. In this study, we combine MD and the Topology Optimization of Binary Structures (TOBS) method approaches for designing nanostructures and nanofluidic systems.

Methodology: The optimisation of nanoscale structures is inherently binary, where a design variable defines the presence of an atom (1) or its absence (0). Therefore, the Topology Optimization of Binary Structures (TOBS) method emerges as a suitable candidate algorithm. Hence, the proposed approach, NanoTO, combines MD simulations with the TOBS method.

Preliminary results: In nanomechanics, the primary achievements are linked to applying NanoTO to optimise the mechanical properties of carbon and metal nanostructures. Other significant breakthroughs have been realised in the realm of nanofluidics. An optimised

nanochannel has been devised using NanoTO to minimise pressure drop.

Preliminary conclusions: This pioneering study seamlessly blends molecular dynamics and topology optimisation to engineer optimised nanostructures and nanofluidic systems, which can substantially contribute to advancing emerging nanotechnologies like nanoelectromechanical systems (NEMS) and membrane technologies. A new path emerges through the fusion of both methodologies, unlocking the potential of nanostructures and nanofluidic systems, thus shaping the future of manipulating solid-fluid interactions at the nanoscale.

Diego Hayashi Alonso
Escola Politécnica da Universidade de São Paulo

Abstract Title: Rotating resonance under low density flow for machine rotor topology optimization

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Abstract: The emission of greenhouse gases is one of the main factors that lead to global warming. One important element in the emission of greenhouse gases are turbomachines (compressors and turbines). By improving their design, they should become more efficient and, therefore, cause less emissions of greenhouse gases for the same operating conditions. Specifically in the design of flow machine rotors, it is important to consider not only the fluid flow performance, but also the resonance phenomenon, since it may lead the whole machine to fail. When under rotating conditions, the formulation and behaviour of the structure changes, which requires a new formulation. Thus, a new topology optimization approach is formulated for rotating resonance considering a low-density fluid flow, which allows some simplifications in the formulation. In the end, there are three different effects, one for each different physics: the modal analysis, the solid structure, and the low-density fluid flow. The topology optimization formulation is given for a simplified 2D model of a rotating fluid flow device. An integer linear programming algorithm is used in the topology optimization approach, and some numerical examples are presented.

Keywords: Topology optimization; Resonance; Low density fluid.

Introduction and Objectives: Global warming is mainly caused by the emission of greenhouse gases. Particularly, turbomachines (compressors and turbines) are an important contributor to it. This means that, by improving their design, they should become more efficient,

leading to less emissions of greenhouse gases for the same operating conditions. Mainly, the design of flow machine rotors requires not only to have a good fluid flow performance, but also to avoid resonance. Resonance is a phenomenon that can easily lead to the failure of the whole device, and should, therefore, be avoided. Previous works in the topology optimization of flow machine rotors only dealt with the fluid flow performance issue (Romero and Silva, 2014) without, however, considering the effect of resonance. Thus, the current work aims to tackle this issue by formulating the topology optimization method for this case. The implementation is to be coupled to the FEniCS TopOpt Foam library (Alonso et al., 2021), in order to couple the efficient CFD from OpenFOAM® with the finite element platform FEniCS and the automatically derived sensitivities from the dolfin-adjoint library.

Methodology: The new topology optimization formulation is given for a low-density fluid flow, structural effects and modal analysis. Also, a simplified 2D model is considered for the flow machine rotor. The fluid flow simulation is computed in the CFD software OpenFOAM® and interfaced with the topology optimization framework by using the FEniCS TopOpt Foam library. The structural simulation, as well as the modal analysis, are performed in the finite element-based platform FEniCS. The sensitivities are automatically computed by using FEniCS/dolfin-adjoint, and, more specifically, the modal sensitivities are composed by hand, since the modal analysis is solved intrinsically different from usual FEM approaches.

Preliminary results: The new topology optimization formulation is demonstrated for the low-density fluid flow through a compressible and an incompressible case, showing the effects of each objective function (fluid, structural and modal) in the flow machine rotor design.

Preliminary conclusions: A new topology optimization formulation was formulated and numerically demonstrated for a low-density fluid flow, by considering compressible and incompressible fluids. The effects of each objective function (fluid, structural and modal) were shown in the flow machine rotor design. In the form of future work, some suggestions would be to consider turbulence, more vibration modes, the gyroscopic effect in the modal analysis etc.

Eduardo Moscatelli de Souza
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Abstract Title: Design of stepped labyrinth seals by topology optimization

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Abstract: Turbomachines present an inherent leakage between rotating and stationary components as these parts may not be in contact during operation. One common design strategy to reduce this leakage is to employ labyrinth seals, which are robust devices that provide a highly dissipative path to the fluid flow. Labyrinth seals are an important technology for reducing greenhouse gas emissions because they are commonly employed in compressors operating with carbon dioxide (CO2) and methane (CH4). Therefore, the optimization of labyrinth seals is of high environmental importance. This work designs stepped labyrinth seals by applying the topology optimization algorithm developed by a partnership between the University of São Paulo (USP) and the Technical University of Denmark (DTU), which was established during the X RCGI Colloquium. Here, the focus is on the stepped labyrinth seal configuration, which presents a misalignment between the inlet and outlet of the seal. The algorithm uses an interface identification technique previously devised to design heat exchangers and a connectivity constraint developed for additive manufacturing. Combining these techniques allows the control of the minimum gap and the assignment of different velocities to the rotor and stator. Also, it avoids solid parts that are not connected to any wall. The key idea is to model the fluid channel as the interface between rotating and stationary parts. The fluid flow and adjoint equations are solved by the finite element method with quadratic, linear and linear triangular elements for the velocity, pressure, and design variable fields, respectively. The optimization problem is solved with the Method of Moving Asymptotes (MMA).

Keywords: Topology optimization, Labyrinth seals, Interface identification method, Virtual temperature method.

Introduction and Objectives: Labyrinth seals are a standard solution to reduce leakage in compressors operating with carbon dioxide (CO2) and methane (CH4). Therefore, they play an essential role in reducing greenhouse gas emissions. Among the labyrinth seal configurations, the stepped labyrinth seal offers a high leakage reduction because the inlet and outlet of the labyrinth seal are not aligned. The objective of this work is to design stepped labyrinth seals with the topology optimization algorithm developed by a partnership between the University of São Paulo (USP) and the Technical University of Denmark (DTU), which was established during the X RCGI Colloquium. The algorithm uses an interface identification technique previously devised to design heat exchangers and a connectivity constraint developed for additive manufacturing. Combining these techniques allows the control of the minimum gap and the assignment of different velocities to the rotor and stator. Also, it avoids solid parts that are not connected to any wall.

Methodology: The fluid flow, density filters and adjoint equations are solved by the finite element method with quadratic, linear and linear triangular elements for the velocity, pressure, and design variable fields, respectively. The FEniCS framework is used to implement the finite element models. The non-linear fluid flow equations are solved by Newton's method (PETSc) and all the linear systems are solved with MUMPS. The optimization problem is solved with the Method of Moving Asymptotes (MMA).

Preliminary results: Stepped labyrinth seals with intricate geometry and high head loss;
Control of the minimum gap of stepped labyrinth seals; Description of the shaft rotation during the optimization of stepped labyrinth seals.

Preliminary conclusions: The interface identification method developed for heat exchangers is capable of asserting a minimal gap for labyrinth seal design;
The interface identification method enables the assignment of different velocities to the rotor and stator during the optimization; The virtual temperature method is capable of avoiding free-floating islands during the stepped labyrinth seal design; The rotation plays an important role during the design of stepped labyrinth seals.

Enrique Vilarrasa Garcia
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Abstract Title: Influence of the SO2 adsorption on CO2 capture from flue gas using 13X zeolite

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Abstract: Carbon dioxide (CO2) capture is a widely studied topic, with Carbon Capture and Storage (CCS) methods gaining prominence, especially processes based on gas-solid adsorption. However, the literature still lacks studies about the impacts of contaminants from gaseous streams (NOx, SOx, humidity, etc.) on the CO2 adsorption. This work aims to study the effects of the presence of SO2 in gas streams on the performance of CO2-adsorbents

Keywords:13X zeolite, flue gas; CCS; SO2.

Introduction and Objectives: Carbon dioxide capture has been widely studied, given the impacts of this pollutant in the atmosphere, and there are several technologies for carbon capture and storage (CCS), such as pressure swing adsorption (PSA), vacuum swing adsorption (VSA), and temperature swing adsorption (TSA) (Yong et al, 2002). It is noteworthy that the efficient performance of adsorption technologies is related to the effect of contaminants present in the gas streams, as these can profoundly impair the performance of the adsorbent. According to Zhang et al., sulfur oxides (SOX) and nitrogen oxides (NOX) are the contaminants that most affect the performance of CCS technologies (Zhang et al, 2016). However, the literature is quite incipient in terms of understanding the effects of SOx and NOx on adsorbent performance and how they affect CO2 capture. Thus, the present work aims to assess the impact of sulfur dioxide (SO2) on CO2 capture from flue gas derived from combustion of biomass References: Yong Z, Mata V, Rodrigues AE, Frias R. Adsorption of carbon dioxide at high temperature-a review. vol. 26. 2002. Zhang D, Wang H, Wang Q, Li W, Jiang W, Huo P, et al. Interactions of nitric oxide with various rank coals: Implications for oxy-coal combustion flue gas sequestration in deep coal seams with enhanced coalbed methane recovery. Fuel 2016;182:704–12. https://doi.org/10.1016/j.fuel.2016.06.018.

Methodology: Commercial 13X binder free zeolite (13XBF) from Köstrolith (Germany) was used as adsorbent. 13X zeolite is commonly used to separate CO2 from combustion gases (Wilkins and Rajendran, 2019), in addition to being considered a standard reference material for adsorption studies (Morales-Ospino et al. 2019). CO2, N2, SO2, CO2/N2 and CO2/SO2 adsorption measurements were collected in a magnetic suspension balance (MSB) from Rubotherm (Germany), aiming to assess the influence of SO2 adsorption on CO2 capacity of 13XBF. Textural properties were determined from N2 adsorption-desorption isotherms at -196 °C using an Autosorb-iQ3 (Quantachrome Instruments, USA).
X-ray spectroscopy data were obtained in a Physical Electronics PHI 5700 spectrometer with non monochromatic Mg Kα radiation (1253.6 eV, 300 W, 15 kV) and multichannel detector The sulfur content was determined by elemental chemical analysis using a CHNS 932 analyzer supplied by LECO (Geleen, The Netherlands). References: Morales-Ospino, R. et al. Assessment of CO2 desorption from 13X zeolite for a prospective TSA process. Adsorption, v. 26, p. 813-824, 2019. https://doi.org/10. 1007/s10450-019-00192-5 Wilkins, N.S., Rajendran, A., Measurement of competitive CO2 and N2 adsorption on Zeolite 13X for post-combustion CO2 capture. Adsorption 2019: 25, 115–133. https://doi.org/10.1007/s10450-018- 00004-2

Preliminary results: The presence of SO2 in the gas stream reduces the CO2 and N2 adsorption capacity of the zeolite, which may be related to the reduction of textural properties due to SO2-adsorbent chemical interactions. Thus, adsorption of SO2, even at low partial pressures, but for a prolonged time (12 hours), leads to a decrease in CO2 adsorption, which is consistent with the deterioration in textural properties. After SO2 adsorption, the micropore

volume of zeolite calculated from N2 adsorption/desorption isotherms at -196°C, reduces 32%.

X-ray photoelectron spectroscopy (XPS) and elemental analysis (CHNS) tests after SO2 contact for 12 hours confirmed the presence of S species on the surface of the adsorbent, mainly elemental sulfur (ca. 20%) and sulfate ions (ca. 80 %), even after thermal regeneration (300 °C for 10 h). Different configurations for sample regeneration after SO2 adsorption were studied. The maximum SO2 recovery by regeneration was at 350 °C under inert gas flow for 10 hours, recovering 31% of the previously SO2 adsorbed.

Preliminary conclusions: The drop in textural properties due to irreversible adsorption of S species, and therefore the selective CO2 capture, did not turn out to be cumulative over the course of adsorption/desorption cycles. After a first drop in CO2 adsorption capacity of ca. 30%, the amount of CO2 adsorbed during the adsorption/desorption cycles remains practically constant, at least during the 10 cycles investigated.

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Abstract Title: Synthesis and characterisation of nanomaterials for application in nanofiltration membranes and recovery of lithium from produced water

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Abstract: One of the challenges in oil and gas production is managing produced water (PW), representing a critical process for exploration and production in underground reservoirs from social, environmental, and economic perspectives. PW is a byproduct of complex composition, including the water previously present in the reservoir during the formation process, the water injected for extraction, and other chemical additives used during extraction. The proper management of the PW is crucial given the significant economic interest and demand for lithium (Li) because of its high technological need in the energy industry and its potential for sustainable resource reuse. This work focuses on researching and developing innovative

technologies utilising nanomaterials with enhanced structural and physical properties. The main objective is to increase the selectivity of Li ions in an aqueous matrix, even in the presence of other monovalent and divalent ions at varying concentrations. To simulate conditions close to

reality, we used a sample of synthetic brine that replicates the concentrations found in PW samples. The selection of samples was based on a multiscale research process in which we explored various two-dimensional (2D) and three-dimensional (3D) materials. Initially, through computational analyses, we identified materials with enhanced selective capacities for Li-ions, minimising interference from common ions such as sodium (Na), typically present in significant concentrations. From identifying the most promising candidates for the Li recovery process, materials with favourable properties were selected for applications in Lithium-ion sieves (LIS), which encompass both 2D and 3D materials, with a special emphasis on their selectivity for Li+ over Na+.

Keywords: Lithium-ion sieves, Synthesis and characterisation, nanomaterials, membranes, nanofiltration.

Introduction and Objectives: This research aligns with current efforts in treating and recovering ions found in produced water (PW), a high-volume byproduct generated during offshore oil and gas extraction processes. Our primary focus is the selective recovery of Li+ ions from a diverse aqueous matrix containing other mono and divalent ions. This endeavour is pivotal for ensuring the efficiency and sustainability of Li recovery processes, ultimately advancing energy storage technology and responsible natural resource management. Due to its growing demand, Li ions have gained substantial economic interest in the energy industry. Identifying and developing nanomaterials capable of selectively capturing Li ions becomes critically important in the current context. This is particularly challenging due to other ions in significant quantities in PW. This approach is vital to ensure the efficiency and sustainability of Li+ recovery processes, thus advancing energy storage technology and responsible natural resource management. The samples chosen for investigation concerning selective Li+ extraction originate from a compilation of studies focused on nanofiltration through Lithium-ion sieves (LIS) and the adsorption energy of Li within various 2D and 3D materials, with an emphasis on their selectivity over Na+, K+, Ca+2 and Mg+2. A spectrum of materials based on ion exchange principles was employed to initiate this investigation. These materials find applications in water softening, industrial chemical purification, valuable metal recovery, and other domains. This phase of material screening is firmly rooted in laboratory experimentation and industrial implementation, highlighting its significance. Among the investigated materials, TiO2 is noteworthy, leading to further investigations into its structure and related compounds like Li2TiO3, which find applications in LIS. Additionally, spinel LMO adsorbents, such as LiMn2O4, Li1.6Mn1.6O4, and Li1.33Mn1.67O4, have garnered increasing attention due to their distinctive spinel structure and intricate three-dimensional network channels. These features give them exceptional selectivity and absorbability for Li+. The compound Li2TiO3,

characterised by a perovskite crystal structure composed of Li+, titanium (Ti+4), and oxygen (O-2) ions, has shown intriguing properties for ion exchange [1-2] and has gained attention in LIS applications due to its high affinity for the crystal lattice compared to alternative materials.

Methodology: The primary objective of this experimental analysis is to identify structural variations within the samples. Specifically, we aim to investigate the potential exfoliation of TiO2/MnO2 nanolayers through acid bath treatment and the creation of vacancies within the three-dimensional structure of Na2TiO3/Li2TiO3/NaMn2O4/LiMn2O4 samples, which are being synthesised via a solid-state reaction. These characterisations will yield vital data for assessing the recovery of Li+ and Na+ ions through the ion exchange process, ultimately enhancing the material's suitability as an effective ion sieve. To achieve these goals, the samples will undergo measurements utilising polycrystalline X-ray diffraction (PXRD), Transmission Electron Microscopy (TEM), and Scanning Electron Microscopy (SEM). These techniques will provide a comprehensive understanding of structural and morphological changes in the samples at various stages: initial preparation, after acid bath treatment, and following the recovery process using a synthetic brine solution. To quantify recovered Li+, we will employ measurements using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-EOS) to assess the synthetic brine ion concentration before and after interaction with the samples. In preparing the synthetic brine solution, we calculated the concentrations of essential elements based on values obtained from a survey of offshore produced waters [3-4]. A critical consideration in determining these concentrations was ensuring alignment with a computationally feasible concentration range, enabling comparison with theoretical calculations. This process began with simple models of the Li+ ion and later expanded to solutions incorporating Li+ along with other ions, including Na+, K+, Mg+2, Ca+2, and chlorine Cl-. The experimental formulations for evaluating Li+ selectivity concerning the presence of other ions were thoughtfully devised in stages. Initially, we prepared solutions containing only Li+ and Cl-. Subsequently, we developed combinations that included the presence of other monovalent or divalent ions. These combinations were expanded to encompass the simultaneous presence of two or three ions from the series.

References:

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Preliminary results: The synthesis of these materials is currently undergoing testing, focusing on assessing their selectivity in capturing Li+ ions. This study will examine their performance across solutions of synthetic brine which have been prepared. The experimental findings will

then be compared with computational data to establish correlations and insights into the efficiency of Li+ capture by the synthesised materials.

Preliminary conclusions: The investigation into selective Li+ extraction from a wide range of 2D and 3D materials highlighted the significance of material screening based on ion exchange

principles. Among the materials studied, TiO2, Na2TiO, Li2TiO3, NaMn2O4 and LiMn2O4, characterised by its perovskite crystal structure, has shown promise for ion exchange applications, particularly in Lithium-ion sieves (LIS). Ongoing efforts are focused on synthesising these materials and evaluating their selectivity in capturing Li+ ions. Also, experimental formulations of synthetic brine were designed to assess the selectivity of Li+ in the presence of other ions. This approach aimed to provide insights into the nanomaterials' capabilities under varying conditions, including ion types and concentrations.

Francisco Hélio Alencar Oliveira
Naval Architecture and Ocean Engineering USP

Abstract Title: GHG reduction through Topology Optimization and Additive Manufacturing

Authors' Names & Affiliation Institutions of all authors: Francisco Helio Alencar Oliveira, Prof. Dr. Emilio Carlos Nelli Silva, Prof. Dr. Renato Picelli, Prof. Dr. Marcos Guerra Tsuzuki.

Abstract: Industry 4.0 demonstrates an immersion in new technologies, which means that, once the industry positions itself in this new context, it plans and invests in research and development to act in a robust and competitive manner. Academia has a primary role as a foundation for basic research since the scenario presents itself with numerous disruptive technologies. Technologies such as the Internet of Things, Augmented Reality, Additive Manufacturing, Cloud Computing, Autonomous Robots, Artificial
Intelligence are called pillars of this industry 4.0 as other platforms are consolidating themselves as 5G technology, thus forming the bases for the so-called “Smart factories” and “ Smart Cities”. Among the sustainable development objectives, the following stand out: Drinking water and sanitation, Clean and affordable energy, Industry innovation and infrastructure and Action against climate change. The construction industry has been adopting initiatives aligned with the challenges of Industry 4.0 and climate change, developing research into new materials and increasingly sustainable processes with a low carbon footprint. The share of cement production in total CO2 emissions has been increasing steadily. It is currently estimated to account for around 8% of total greenhouse gases (GHG). In Brazil, low productivity is due to the high rate of waste of around 30%, together with the waste generated and not reused of 50%. Concrete is used on ships, offshore LPG processing platforms, offshore

wind turbine platforms – FOWP, etc. Automated systems in order to meet the demand for efficiency in production processes, AM has become increasingly widespread, whether in solutions on construction sites or in warehouses equipped with logistics systems. The construction of civil structures through AM provides not only agility in the process, and reduction of raw material waste, but also freedom of form, which provides the use of new design techniques such as the use of MOT to obtain optimal structures, eliminating material addition

in regions of low structural stress, such as the bridge design below designed by topology optimization and manufactured by MA.

Keywords: Additive Manufacturing.

Introduction and Objectives: The Potential of the Additive Manufacturing to revolutionize the construction industry, reduce waste and make it more sustainable. With its ability to create precise and accurate structures through digital fabrication. Use Topology Optimization Methods to develop lightweight structures. Use of sustainable and recycled materials.

Methodology: Consist to implement a systematic process to design the mechanical or civil structures. The use of methods of finite element, topology optimization and additive manufacturing consolidate the state of the art in the design process.

Preliminary results: Topology Optimization method reduced the total weight about 40% in comparison with traditional method., it will reflect also in more productivity to process less material volume consumption.
Preliminary conclusions: The use of AM and TOM reflects more productivity in the process, reducing material consumption, energy and drastically the waste contributing to the reduction of greenhouse gases.

SHORT ORAL SESSION B

10h10 – Short Oral Session B
0811 – SRS5 (TV1)

Chair: Edmilson Moutinho dos Santos – Sigmar Malvezzi

Allan Yu Iwama
Oceanographic Institute, University of São Paulo, São Paulo, Brazil

Abstract Title: Ecosystem-based management as an approach to assessing the social-environmental impacts of offshore wind energy

Authors' Names & Affiliation Institutions of all authors: Allan Yu Iwama - Oceanographic Institute, University of São Paulo, São Paulo, Brazil; Luciana Yokoyama Xavier - Oceanographic Institute, University of São Paulo, São Paulo, Brazil Ivan Rodrigo Abrão Laurino - Oceanographic Institute, University of São Paulo, São Paulo, Brazil; Marcia Regina Denadai - Institute for Advanced Studies, University of São Paulo, São Paulo, Brazil; Carla Grigoleto Duarte - Federal University of São Paulo, Diadema, Brazil; Ana Paula Alves Dibo - Politécnica School, São Paulo University, São Paulo, Brazil; Luis Enrique Sanchez - Politécnica School, São Paulo University, São Paulo, Brazil; Alexander Turra - Oceanographic Institute and Institute for Advanced Studies, University of São Paulo, São Paulo, Brazil.

Abstract: Offshore wind farms hold promises for Brazil's green transition with over 78 projects marked on the Offshore Wind Complexes map, highlighting the nation's growing interest. However, the impacts of offshore wind farms on Brazilian biodiversity and ecosystem services necessitate further research. This proposal seeks to develop a theoretical-methodological approach for impact assessment based on Ecosystem-Based Management (EBM) principles, tailored to the Brazilian coastal zone. Key inquiries driving the EBM design involve refining regulations, understanding cumulative impacts on the offshore environment's social and environmental components, elucidating biodiversity elements influencing ecosystem processes, exploring traditional ecological knowledge, and leveraging digital tools for disseminating knowledge on regional-scale impacts. With this approach, we aim to unveil causal chains between cumulative impacts and ecosystem services implications, essential for guiding Brazil's energy transition. The approach emphasizes a holistic integration of marine spaces, biodiversity, and societal aspects in a systemic and transdisciplinary framework. The envisioned outcome is to provide foundational elements guiding area-based management, such as marine spatial planning, towards coastal-marine public policies for a sustainable energy transition while ensuring the continued provision of essential ecosystem services.

Keywords: Ecosystem-based management, offshore wind, energy transition, ecosystem service.

Introduction and Objectives: Concerns about climate change have reinforced discussions and initiatives towards transforming the energy matrix from fossil fuels to renewable energies to reduce the GHG in this matrix base. The Energy Transition, as it has been called, has encouraged renewable sources, such as wind, solar, bioenergy, and others (green-blue hydrogen, hydraulic power).

In Brazil, the offshore wind farms have an estimated potential of generation of 700 GW, considering waters up to 50 meters deep and winds above 7 m/s. It is considered one of the great promises of the green transition in the medium term (EPE, 2020). In July 2023, 78 projects are listed as ongoing environmental licensing processes at Ibama, the institution responsible for environmental licensing in Brazil (IBAMA, 2023). There are potential impacts of offshore wind farms on biodiversity and ecosystem services recognized in the literature (e.g. changes in seabed habitats and hydrodynamics; changes in trophic webs; barrier effects or displacements; mortality, injuries and behavioral effects associated with vessels and underwater noise; pollution; modified social perceptions and others - Mauricio Hernandes C., et al 2021), the impacts of the offshore wind farm in Brazil are still incipient and needs more research. Furthermore, the lack of regulation of marine spatial planning instruments, known as Marine Spatial Planning (MSP), indicates the need to guide efforts towards studies that indicate how to apply instruments that allow an integrated analysis of ecological and social systems (Boussarie et al., 2023) in the context of offshore wind farms. In this context, the objective of this proposal is to design a theoretical-methodological approach, based on the Ecosystem-Based Management (EBM) framework (Long et al., 2015), bringing ecological, social and governance principles at temporal and spatial scales appropriate to the local and regional context in the case of offshore wind farms in the Brazilian coastal zone. In this approach, we seek to characterise impacts of offshore wind projects and their possible implications on vital ecosystem services, such as: water provision, food provision, or support for the maintenance and functioning of ecosystems, regulation, to ensure balance in hydrological cycles, and cultural services, with benefits for tourism, cultural identity, and intangible aspects (e.g. spirituality, ancestral memories). The key-questions to design the EBM are:

- How are the key EBM principles considered in EIAs and regulations?
- What are the main social and environmental components related to cumulative impacts in the offshore environment?
- Which elements of biodiversity directly affect its ecosystem processes and services?
- How does traditional ecological knowledge relate to SE provision, regulation, cultural aspects?
- How can digital tools amplify the knowledge and share the social and environmental impacts on a regional scale?

Methodology: This proposal is based on This methodology encompasses a multidisciplinary approach, incorporating literature analysis, biodiversity assessments, field studies, social engagement, traditional ecological knowledge integration, and technological tools.

1. Literature Review and Regulatory Analysis To address the first research question regarding how key EBM principles are considered in regulations, a literature review will be conducted. This review will encompass academic papers, government regulations, policy documents, and relevant reports and environmental assessments. To identify the presence or absence of EBM principles we will adapt the method applied by Guilhon et al. (2020) and Xavier et al. (2022).
2. Social and Environmental Component Analysis Review of environmental legislation of offshore energy in selected countries. The main product is a summary of key regulations relative to environmental impact assessment, marine spatial planning and project environmental management and follow-up, including a summary comparative table and a set of best regulatory practices applicable to the Brazilian context. Selected environmental impact studies and other documents pertaining to projects in the selected countries will be reviewed, alongside an extensive literature review. The key products are: (i) standard lists of activities, environmental aspects and impacts, and corresponding mitigation, with corresponding explanatory notes, and (ii) a review of the extent to which cumulative impacts are addressed. 3. Biodiversity Assessment: A review and spatial analysis of marine biodiversity from documents of literature to elaborate the basis of biodiversity in the coast of Brazil
4. Traditional Ecological Knowledge (TEK) Integration To understand the relationship between traditional ecological knowledge and socio-ecological provisioning, regulation, and cultural aspects (fourth research question), interviews and workshops with local communities and indigenous groups will be conducted. TEK will be integrated with scientific knowledge through participatory approaches. Comparative analysis will be performed to understand the contributions of TEK to sustainable management and policy formulation.
5. Digital Tools and Geographic Information Systems (GIS) Review of digital tools and Spatial Data Infrastructure (SDI) and GIS to compare and elaborate a review about the importance of geovisualization of environmental and social impacts of offshore winds farms. 6. Integration and Synthesis The final step involves integrating insights from all research components to design the Ecosystem Based Management (EBM) framework. Data synthesis, comparison, and integration will be performed to establish causal relationships, develop a comprehensive understanding, and formulate key elements essential for EBM design.

Preliminary results: With this proposal, we expect to identify best-practices and develop guidelines to support the development of an Ecosystem-based Approch to Environmental Impact Assessment model for offshore wind power development specific to the environmental and social context of the Brazilian coast.

Preliminary conclusions: This ecosystem-based operating model seeks to relate causal chains between cumulative impacts and implications for the main ecosystem services mentioned above. Therefore, analysing offshore wind farms, in the context of an important energy transition for the country, requires integrating the space marine environment with biodiversity and social aspects, in a systemic and transdisciplinary perspective. We expected that our EBM design offers key elements to support the MSP to focus on coastal-marine public policies, aiming to provide foundations for an energy transition that guarantees essential ecosystem

services for life.

Guilherme Porfirio Baccari
Institute of Psychology of University of São Paulo

Abstract Title: Risk perception associated with Carbon Capture and Storage technology in Brazil: a comparison between experts and non-experts.

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Abstract: In order to mitigate the effects of climate change it is necessary to employ every strategy and technology available. And one of the most promising in the global scene is Carbon Capture and Storage (CCS). Such technology, however, faces many challenges in its implementation, among them a highly negative social perception which led many projects to be canceled. Aiming to understand such negative perception we use the lens of Social Psychology, the science that studies the relationship between the individual and the group. Through a literature review it was found that among the most prominent factors that shape social acceptance is the perception of risks and benefits associated with CCS. So, to study how the perception of such risks occurs in Brazil, we used the Q-Methodology, a qualitative and quantitative methodology especially useful to study the narratives and the social representations relative to a subject. We applied the methodology with experts and non-experts, mostly professors and students in the University of São Paulo. We hypothesize that low levels of knowledge among non-experts influences the risk evaluation, that despite a high consciousness regarding climate change in brazilians, shapes negative perceptions. Experts, otherwise, tend to minimize technical risk evaluation and disregard risks related to the social aspects of CCS implementation such as job and economic dynamics. Therefore, we expect diverse narratives and different social representations about CCS in between experts and non-experts.

Keywords: Carbon Capture and Storage, Q-Methodology, Risk Perception, Social Perception, Social Representation, Narrative.

Introduction and Objectives: Carbon Capture and Storage (CCS) is a relatively new technology that aims to fight climate change by reducing the greenhouse gas emissions by capturing CO2 from industrial and energy power plants and storing it mainly in depleted oil, gas and saline formations. Despite the technology's potential to be responsible from 15 to 55% of global efforts against climate change up to 2100, according to the IPCC, its implementation is still disputed in the public arena. Historically many CCS deployment projects have been cancelled due to bad public opinion and contrary manifestations, some are worth mentioning such as Barendrecht in the Netherlands, Beeskow in Germany and Carson in the United States,

resulting in the loss of thousands of dollars and years of effort. Therefore, in order to understand the public/social opposition and acceptance of such enterprises, the Social Sciences and among them Social Psychology have leaned over the subject for the past ten years. In such way literature found many factors that link the individual and the group and explain, at least partially the social perception and acceptance regarding renewable energy and sustainable technologies, some such factors are sense of community empowerment, Not In My Backyard effect (NIMBY), previous history with oil and gas industry, communication, trust in the agents involved, knowledge about CO2 and CCS, awareness of climate change, perception of tampering with nature, fear of leakage and explosion; however, the most studied factor and one of the most relevant is the risk perception (and its counterpart, the benefits) of CCS deployment. Then, based on the literature, our objective is to research the social perception regarding the risks associated with CCS deployment in Brazil, evaluating the narratives and social representations constructed in the social tessiture and taking advantage of our position in a renowned research centre (RCGI) where many experts in CCS work and study, we aim to compare the perception of risk between experts and non-experts. This way we intend to contribute to the enhancement of this research field in Brazil and pave the way for more complex studies.

Methodology: Our chosen methodology is the Q-methodology, developed by physicist and psychologist William Stephenson in 1935. Q is a qualitative and quantitative approach that studies subjectivity through objective means, it is ideal to study the social representations of such theme and the narratives concerning it. We chose this methodology because the vast majority of literature on social perception of CCS uses only surveys, questionnaires and (lesser times) focal groups or interviews, there are few articles that use mixed methods. Besides, it allows us to access the many narratives about CCS implementation with one unique, but carefully constructed, instrument saving time and resources. Q methodology's main research process is the application of a set of cards with affirmations, that is the concourse, which is carefully constructed based on literature, interviews and other readings and contains everything spoken about a theme. The participants, then, must reorder the cards with the affirmations from less likely their way of thinking to most likely. In our case affirmations are about the risks related to CCS implementation, in order to form a quasi-normal structure and in this way answer a question made by the researcher. A follow-up interview is made in order to access and clarify the logic for the composition. Then, summing up the composition of all participants, Q-methodology proposes a factorial analysis based on the affirmations and comprises then in group factors that represent different points of view regarding a theme. Finally it is up to the researchers to form the narratives underlying the grouped factors, using as complementary sources the interviews and the literature review. In our research we plan to apply the Q-methodology to 10 experts and 10 non-experts using a 63-card deck containing affirmations about CCS risk perception divided in 7 artificial categories of statements: risks related to the involved agents, risks related to the steps of production/implementation of CCS, local risks and socioeconomic factors, global risks and factors, risks related to the environment, risks related to psychological factors and associations related to CCS.

Preliminary results: our expected results are: a) the formation of different narratives and social representations regarding the risk perception of CCS implementation in Brazil, b) accentuated differences between the experts and non-experts' group, where c) experts would tend to dismiss social risks because of their distance to the field, as well as d) present lesser technical risk perception because of their knowledge. Also, we expect, in accordance to the literature, e) low levels of knowledge among non-experts about CCS, even in university students, that lead to f) high levels of CCS implementation opposition, despite g) high levels of climate change awareness. Also, for locals h) social/local problems may be seen as more important than the one caused by climate change, increasing the risk perception and low perception of CCS benefits.

Preliminary conclusions: Our modest conclusions are that the CCS implementation in Brazil shall face difficulties in regarding the social perception of it. As the technology may be seen as an end-of-the-pipe solution and a way for oil companies to greenwash their activities. Furthermore, we indicate a distance in between the representations of CCS risk in experts (plus agents involved in the project deployment) and non-experts (plus locals residing the deployment region), so we recommend that companies employ transparent communication with local communities, envolve then in the decision making process, as well as generate clear benefits such as jobs, payments for the land use, investments in the health and/or infrastructure systems of the region, and have a compensation policy.

Gustavo Chagas de Morais
University of São Paulo

Abstract Title: Molecularium: Immersive Experiences for Scientific Dissemination

Authors' Names & Affiliation Institutions of all authors: Gustavo Chagas de Morais University of São Paulo, University of São Paulo.

Abstract: Climate change presents a pressing global challenge with far-reaching impacts, many of which unfold at a microscopic, molecular scale. These intricate phenomena remain hidden from the naked eye, making it challenging for the public to grasp the complexities of climate science. This project employs immersive experiences, specifically virtual and augmented reality technologies, to bridge this comprehension gap. The project centres on Molecularium, which allows interactive, virtual reality-based explorations of climate-related molecular phenomena. These immersive experiences offer a tangible perspective of climate change intricacies, effectively altering the public's perception of scale and fostering a deeper connection with the subject. The research aims to assess the educational and dissemination impact of these

immersive tools. The project uses classical molecular simulations to create interactive virtual reality experiences that allow participants to delve into the molecular world. Real-time sound enhancements via sonifications add depth to these interactions, enhancing comprehension.
These advanced simulations have been showcased to diverse audiences, including the public, research groups, and educational institutions, receiving recognition at thematic events. The next phase involves comprehensive data collection across various demographic groups. This data will measure immersion levels, assess the Molecularium's effectiveness as a learning tool, and evaluate the impact of virtual reality on comprehending climate change-related concepts.

Keywords: Dissemination, virtual reality, communication, molecular dynamics.

Introduction and Objectives: The project is dedicated to introducing the challenge of climate change to the public using immersive experiences, specifically focusing on virtual and augmented reality technologies. Within this context, a big part of the related phenomena manifest on scales significantly different from the planetary scale, often occurring at the molecular level. The project team proposes using visualisation tools and sensory aids to portray these phenomena realistically.
The Molecularium serves as the epicentre of the research, functioning akin to a molecular planetarium. This platform enables the interactive deployment of virtual reality tools to present and discuss molecular phenomena, offering a perspective aligned with a low-carbon society. A fundamental aspect of this endeavour is assessing these immersive tools' didactic and dissemination impact.

Methodology: The Molecularium utilises computational simulations of classical molecular dynamics to facilitate interactions in virtual reality. These interactions are rendered using the Unity and UnityMol graphics engines connected to a server. The interactions with molecular systems in virtual reality trigger calculations that influence the molecular dynamics of these systems. Using the same server, immersive experiences can be extended through sound, employing sonifications to convert system parameters into real-time sound, thus enhancing and presenting aspects of the system during physical interaction. These interactions are conducted using virtual reality headsets such as the Oculus Rift at controlled stations, emitting three-dimensional sounds. These experiences are presented to the public at events, serving as case studies. In those, collecting data for developing the platform as a science dissemination tool and public perception mapping is possible. In line with the data collection effort, an in-depth questionnaire is under development, focused on assessing several key aspects: the level of immersion participants experiences during the virtual reality simulations, gauging the potential of the Molecularium as a practical learning tool and evaluating the impact of virtual reality on participants' comprehension of complex climate phenomena.
Preliminary results: Significant progress has been achieved in developing virtual reality simulations over the last few months. These interactions now offer full functionality in both interactive and passive formats. These approaches reach the potential to comprehensively measure immersion levels and assess their impact on participants' understanding of climate

change-related phenomena. Moreover, these advanced virtual reality simulations can be integrated into other products with content related to various phenomena associated with a low-carbon society, such as CO2 mineralisation, gas separation, and CO2 catalysis. Furthermore, these advanced virtual reality simulations were presented to diverse audiences, including the public and research groups, at various RCGI and IFUSP cores events. They have also been showcased during educational visits to schools and across multiple disciplines at the Institute of Physics at USP and the USP Escola. Additionally, the project gained recognition at thematic events about low-carbon society and science communication.

Preliminary conclusions: As the project advances, the forthcoming semester presents an opportunity for more extensive data collection involving a diverse spectrum of participants, including primary education students, teachers, undergraduates, and researchers. This comprehensive phase is expected to yield substantial insights, offering concrete metrics to assess the impact of varying immersion levels on public engagement and comprehension of the main topics. Additionally, virtual and physical versions of the Molecularium (Digital Lab and Inova USP) are being promoted for dissemination to the public, extending the reach of experiences and engaging with more diverse audiences. Other aspects that may come with the data involve determining virtual reality's educational impact beyond its entertainment appeal. So, it is essential to distinguish whether the positive responses from different audience segments are primarily due to the technology's novelty or novelty factor, or if they signify meaningful learning experiences. This nuanced understanding will help shape future refinements, ensuring that the project effectively addresses a variety of the Molecularium specifics needs and interests across a different audience and, based on the conclusions regarding the novelty of the platform, there may be an opportunity to focus on a more targeted audience rather than a broad one.

Ricardo Pagio Betini
University of São Paulo (USP).

Abstract Title: How can personality influence perception and behavior towards climate change? An exploratory study

Authors' Names & Affiliation Institutions of all authors: Ricardo Pagio Betini- IPUSP, Karen Mascarenhas - RCGI USP.

Abstract: The perception of climate change is modulated by several factors that are widely discussed and systematized over time by different studies. In this sense, the influence of personality on how people interpret and respond to environmental problems and the development of low-carbon technologies is a relevant and complex topic. One of the most consolidated theories regarding the constitution of an individual's personality, The Big Five

traits or factors (or Five Factor Model), places this construct as being made up of five dimensions or domains, which are Openness, Conscientiousness, Extraversion, Agreeableness, and Neuroticism. Taking this into account, the study has an exploratory nature to understand how the five traits described in the model are constituted and reflect attitudes and beliefs regarding climate change. To do this, a bibliographic search will be carried out containing keywords that filter articles already produced on the topic in the ScienceDirect platform database. For each of the five traits, the frequency with which they appear in greater or lesser intensity for pro-environmental behaviours and the particular differences between each group that contains the same characteristics will be sought. The expected results of this study may indicate that people with high openness and consciousness scores are more likely to perceive climate change as an important problem. In neuroticism, the higher the score for this trait, the more concerned they are about risks and negative impacts. It is important to highlight that although personality is an important factor in the formation of perception, it is only one of the modulators within other social, cultural, educational and economic factors.

Keywords: Personality; Big Five; Climate Change; Environmental Engagement.

Introduction and Objectives: Although acceptance of climate change has increased in recent decades, the challenge of strengthening engagement in actions aimed at mitigating the problem and more effective measures to be taken by society in general remains. Among the various factors responsible for modulating perception, the constitution of the individual's personality is included. The impact of this construct on the social perception of environmental problems and climate change is investigated in several studies. This research demonstrates that different personality traits can shape people's attitudes and reactions to environmental issues and issues related to the acceptance of low-carbon technologies. The Big Five theory, also known as the Big Five Personality Factor model, describes that human personality can be described in five fundamental traits: Openness, Conscientiousness, Extraversion, Agreeableness and Neuroticism. Each of these traits can influence the perception of climate change in different ways. Therefore, the objective of the research is to identify how these traits are distinctly conveyed in people's pro-environmental behaviour and engagement in relation to climate change and carbon mitigation technologies, such as CCS or hydrogen-based technologies.

Methodology: The research is exploratory in nature and will use scientific articles already published for bibliographical research. The database will be from ScienceDirect and the articles will be searched using the keywords “personality”, “Big Five”, “climate change” and “perception”. After surveying these articles, a preliminary analysis of their abstracts will be carried out to identify whether there is a correlation with the researched topic or not. After selecting the articles that meet the objective of this research, the analysis will focus on the results of each study. To this end, the main information will be sought that relates solely to the five traits of the theory used here, and how they are present in the different groups studied.

Preliminary results: Although there are still no robust results from the research, some inferences are possible to make given previous readings. Neuroticism, a trait associated with the tendency to feel anxiety and worry, would be associated with greater concern about climate change. This means that the higher the score for this trait, the more likely they are to feel distressed by environmental threats and, therefore, the more likely they are to perceive the severity of climate issues. Regarding conscientiousness, highly conscientious people tend to be more disciplined and goal-oriented, which can lead them to take steps to reduce carbon emissions and promote sustainability. Extraversion, a trait related to sociability and orientation toward others, may influence perceptions of climate change through social norms. Agreeableness is related to empathy and consideration for others. People high in agreeableness may be more concerned about the effects of climate change on vulnerable communities and biodiversity. In relation to openness, further study of the trait is needed to provide more precise statements, as there is not a very tangible pattern based on the results of the articles that have already been read. Preliminary conclusions: The way in which personality traits can elicit pro-environmental behaviours is fundamental to a more complete understanding of how an individual is able to relate environmental impacts to their own internal functioning structure. It is worth highlighting that despite the importance of this construct for better understanding attitudes and beliefs, other factors are also necessary to be evaluated and analysed in the formation of social perception of climate change. The RCGI project 70 group itself has already mapped these factors in a broad literature review. Psychological factors are addressed in many studies on social perception of climate change. However, the impact of personality using the big five model does not yet have a large number of disclosures on a more consolidated basis, despite the importance of this theory for understanding human personality. Therefore, it is necessary that more research be carried out with populations from different countries and regions of the world, so that a real portrait of the diversity of personalities around the globe can be expressed.

Preliminary conclusions: The way in which personality traits can elicit pro-environmental behaviours is fundamental to a more complete understanding of how an individual is able to relate environmental impacts to their own internal functioning structure. It is worth highlighting that despite the importance of this construct for better understanding attitudes and beliefs, other factors are also necessary to be evaluated and analysed in the formation of social perception of climate change. The RCGI project 70 group itself has already mapped these factors in a broad literature review. Psychological factors are addressed in many studies on social perception of climate change. However, the impact of personality using the big five model does not yet have a large number of disclosures on a more consolidated basis, despite the importance of this theory for understanding human personality. Therefore, it is necessary that more research be carried out with populations from different countries and regions of the world, so that a real portrait of the diversity of personalities around the globe can be expressed.

Miguel Vera Moreno
Instituto de Física da Universidade de São Paulo, IFUSP, São Paulo-SP, Brazil

Abstract Title: A Citizen Science Approach to improving public perception of low-carbon society: A Sentiment Analysis

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Abstract: Citizen science involves the public collecting scientific data using Internet-based technologies, promoting online communities. Social networks, particularly Twitter, improve this commitment by facilitating debates and providing access to much information. Twitter data is analysed to measure public sentiment about climate change. Furthermore, the Natural Language Process, specifically the BERT architecture, classifies feelings in Portuguese tweets. This project aims to predict public opinions on climate change through time series analysis. It is part of the Advocacy program of the Research Center for Innovation in Winter Effect Gases, emphasising the convergence of civic science, social networks and AI.

Keywords: Twitter; sentiment analyser; machine learning; BERT.

Introduction and Objectives: Citizen science is an engaging strategy that enlists the public in gathering scientific information. Internet-based technologies have facilitated large numbers of volunteers contributing to scientific projects. The general public can contribute by collecting data, mapping how environments evolve, and expressing ourselves as never before. This conversational approach has significantly contributed to developing, establishing and nurturing online communities. Social media can be defined as a set of online tools designed to enable and promote social interactions. This media has revolutionised how we communicate with others and share our daily experiences and opinions. However, there needs to be more understanding of how social media may contribute to citizen science in the context of open data sources such as microblogging platforms. One of the most common is Twitter, an available social media platform. Twitter supports the conversational nature of discussions, providing easy access to a wealth of information and data. These data can be a powerful source of insights on various topics, including specific issues like climate change. In recent years, Twitter has gained significant interest from the research community. Sentiment analysis of tweets has emerged as a hot research topic. However, analysing sentiment with multiple classes has proven to be a challenging task. This is mainly because a tweet often contains not just one but multiple sentiments. This work uses Twitter data to map the public perception of climate change and

energy transition issues. We introduce a novel approach for automatically classifying the sentiment of Twitter messages in Portuguese. Machine learning techniques and tools for sentiment analysis are applied to unveil the social pressure and tendencies on the public perception towards low-carbon technologies. To enable computers to understand human language, both written and spoken, we employ Natural Language Processing (NLP), a subfield of Artificial Intelligence. An example of our practical application is sentiment classification in sentences, such as Twitter texts. Within Natural Language Processing, the BERT (Bidirectional Encoder Representations from Transformers) architecture has garnered significant developer attention. It is currently regarded as the most efficient Machine Learning model in this field. The BERT architecture may be key to providing real solutions for present and future needs. Based on this, our work involves classifying Portuguese tweets using the BERT architecture. We take advantage of the enormous amount of text data extracted as positive and negative, and we can carry out a time series study to make predictions about public opinion concerning climate change. This project is part of the Advocacy program at the Research Center for Greenhouse Gas Innovation.

Methodology: This work uses Twitter data to map the public perception of climate change and energy transition issues. For this, it is necessary to carry out sentiment analysis. This is performed to rank sentences using machine learning algorithms. This means that we will analyse the polarity expressed in the messages published on Twitter. To carry out the analyses, we used the Natural Language Toolkit (NLTK) guide package for all NLP tasks (Haseena. et al.,2014). Natural Language Processing (NLP) is a sub area of Artificial Intelligence that aims to make computers capable of understanding human language, both written and spoken. The programming language used to carry out this work is Python. It offers high-level tools, a simple-to-use syntax, and Anaconda as a development environment because it is the right way to install machine learning tools. The work was carried out in two stages. The first step involves creating a database of tweets related to climate change and pre-processing the collected data. The second step is associated with the analysis method, applying machine learning techniques to validate the results. This Section shows the actions performed from the pre-processing phase to the analysis phase.

Preliminary results: After completing the methodology steps, the classification algorithms and analysis of the results were carried out. In the first step of sentiment analysis, tweets were analysed by various sentiment analysers to determine the accuracy of these analysers. The sole purpose of using a variety of sentiment analysers, such as VADER and BERT, was to compare their accuracies. We can see that the accuracy using the BERT algorithm was 85% while using VADER was 90%. VADER was better, but an advantage of BERT is that it was trained with a database already labelled in Portuguese, while VADER is only limited to classifying the text by adding weights to the words. In this case, VADER has a limitation: it considers newspaper tweets as positive or negative. In contrast, with Bert, it is more personalised data, extracting information richer in knowledge. With this classification, it is clearer to create and develop

more efficient time series models that allow us to predict public opinion more precisely.

Preliminary conclusions: This work developed a dataset for sentiment analysis in Portuguese

using Twitter messages. This dataset can serve as a basis for new research and applications in sentiment analysis in our language. On the other hand, we can say that feelings can be predicted more accurately using Machine Learning algorithms, especially logistic regression and linear SVC and Deep Learning like BERT. These have found their use in Natural Language Processing, especially in Sentiment analysis or to determine subjective information like opinion and emotion within a text. However, the accuracy with which each can predict the sentiment varies. As more messages were collected than those classified as future work, more tweets were classified to increase the size of the data set. Another of our significant results was the study of a prediction model that was carried out based on statistical physics approaches. This approach is known as sociophysical. We can see that the concepts of sociophysics can efficiently help to solve more fundamental problems and that they are a powerful tool when applied.

Nelber Ximenes Melo
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Abstract Title: A Philosophical Framework for Sustainable Energy Planning

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Abstract: The increasing energy dependence associated with the severe environmental impacts resulting from natural resource exploitation has triggered a significant race for sustainable solutions for economic and technological development. Simultaneously, as the human population grows, especially in the southern hemisphere, access to technology on this side of the world is also increasing, which may point to a scenario of significant growth in electricity demand in the next 50 years. Furthermore, technological development has fueled urban growth, and digital communication technologies, in particular, have transformed culture, social relationships, and space usage. Overall, these changes further reinforce the trend of increased energy dependence. Typically, the solution to the increasing trend of energy dependence in the context of extreme environmental risk has been to invest in the exploration of new renewable energy sources. As a result, there is an increase in the complexity of technological solutions and their relationships with the environment, given the diversity of different types of energy resources involved, as well as the relationships of technology with society and culture. Nevertheless, traditional energy planning only concerned itself with the technical and economic dimensions of energy resource exploitation. In recent decades, given the recognized ongoing

environmental crisis, a new dimension has been added to energy policies and incorporated into energy planning - the environmental dimension. Nonetheless, energy exploitation, like any technological endeavor, as it constitutes an intervention that transforms reality, not only physically but in its many aspects and relationships, needs to be analyzed in a broader and more detailed manner, under the risk of harming energy justice, social and environmental responsibility, or technical and economic infeasibility. Issues like these have been the concern of scholars in the Philosophy of Technology, a field of study that provides tools for thinking about technology more broadly, including its ontology, analysis, design, and ethics. In this work, the authors seek to apply the philosophy of technology to construct a framework that enables the mapping of the minimum aspects to be considered in energy planning in a way that proceeds with a commitment to the ethics of responsibility and social justice without compromising technical and economic viability. The authors also aim to highlight the potential use of multi-criteria analysis tools in energy planning that align with this orientation.

Keywords: Energy Planning; Sustainability; Philosophy of Technology; Multi-criteria Evaluation.

Introduction and Objectives: Technological activity, which includes energy exploitation, is characterized by intervening in reality to modify it. This intervention may aim to manipulate the existing reality to serve the purposes of human survival and needs, guiding or redirecting natural processes, or even bringing something entirely new into reality or revealing latent meanings present in nature. In this way, technology is developed and used by humans to modify the physical reality, potentially causing irreversible changes in natural processes. The exploitation of natural resources for various purposes, including energy, is therefore an intervention in the environment that can have both positive and negative impacts, or both. Depending on the type of intervention, its intensity, and frequency, these changes may or may not be reversible, either in the long term. According to Crutzen, the Anthropocene is the geological period characterized by the greatest human technological activity, i.e., the greatest human intervention in the environment, especially since the Industrial Revolution. This period is marked by significant environmental impact, from the rapid loss of biodiversity to the biochemical and thermodynamic imbalance of the troposphere, primarily associated with the high emissions of greenhouse gases from technological processes, especially the exploitation of fossil energy resources. However, since reality is multifaceted and not just physical and concrete, the intervention of technology in reality must be considered in all possible aspects that can be analyzed. A justified and deemed necessary intervention in the physical environment can trigger unwanted physical reactions and even non-physical reactions, such as ethical, moral, psychological, or political issues, among various other different natures. Therefore, it is necessary for technological development and, consequently, the exploitation of energy resources to be planned by considering as meticulously as possible all aspects of reality involved in the entire process, as well as all parties involved, interested, or affected by technological action. This work aims to present essential characteristics for responsible and sustainable energy planning, while also being economically viable, using tools from the

philosophy of technology and multi-criteria decision analysis.

Methodology: After identifying the main problematic issues related to technological development and the exploitation of energy resources, the philosophical justification for proposing an energy planning methodology was based especially on the Principle of Responsibility proposed by philosopher Hans Jonas and the virtue ethics of Alasdair MacIntyre. The analytical framework of Herman Dooyweerd was adopted as the basis for mapping the aspects of the complex reality involved in the process of energy resource exploitation. Finally, a study of tools used in other problems involving multiple criteria and stakeholders was conducted, identifying those that could facilitate the implementation of the proposed planning model. A test problem was devised to apply the methodology, namely, the selection of priority renewable sources to be implemented to meet the energy demand of a specific yet-to-be-determined location.

Preliminary results: As preliminary results of the research, through multidisciplinary literature review, the necessary characteristics for an appropriate model of energy planning that encompasses sustainability and responsibility requirements were recognized. Additionally, the philosophical framework that can serve as the foundation for the research implementation was identified, along with potential multi-criteria analysis tools that can assist in the decision-making required for energy planning.

Preliminary conclusions: Herman Dooyweerd's Multimodal Analysis was chosen as the philosophical theory to map the necessary criteria for a sustainable and responsible energy planning to be applied in the process of selecting the priority renewable energy sources for a yet-to-be-determined location. The ANP (Analytic Network Process) model, combined with DEA (Data Envelopment Analysis), was assessed as suitable for weighting the criteria adopted to evaluate the alternatives.

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Abstract Title: Congress and Energy Transition: How the interests of the oil and gas sector are represented in the Brazilian Legislative

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Abstract: This study explores how the interests of the oil and gas sector are represented in the Brazilian Congress. Specifically, it examines how congressmen who are affiliated with parliamentary fronts supporting the oil and gas industry have addressed the topic of energy transition in their proposals, votes, speeches, and statements. To achieve these objectives, Content Analysis, assisted by Atlas.ti software, will be employed. The hypothesis underlying this study is that congressmen aligned with the interests of the fossil fuel sector may have worked to obstruct initiatives aimed at a swift transition to cleaner energy; however, they did not ultimately succeed due to the low level of association and efficiency of the parliamentary fronts in defence of the sector.

Keywords: Parliamentary Fronts, Brazilian Congress, Oil and Gas, Energy Transition, Content Analysis, Atlas.ti.

Introduction and Objectives: The purpose of this study is to explore how the interests of the oil and gas sector are articulated in the Brazilian Congress. It specifically examines how the issue of energy transition has been addressed by congressmen connected to parliamentary fronts that have promoted the oil and gas agenda during current and past legislatures both in Senate and in the Chamber of Deputies, such as the Parliamentary Front for the Sustainable Development of Oil and Renewable Energy, the Parliamentary Front in Support of Oil, Gas and Energy, the Parliamentary Front in Defence of Oil-Producing Municipalities, and the Parliamentary Front for Natural Resources and Energy. We want to achieve this by looking at the votes, stances, speeches, and statements that legislators made from 2010 to 2023 about decarbonisation and the energy transition, with a focus on those from congressmen who are members of parliamentary fronts connected to the oil and gas business. Given the rising demand

for emissions reduction in Brazilian society and Brazil's international commitments, we also seek to understand how these fronts and congressmen have interacted with the ideas of decarbonization and energy transition and to identify any alternative strategies that they may consider.

Methodology: To pursue our research question, we will employ Content Analysis, supported by Atlas.ti software. Content Analysis is a methodology that can take either a predominantly quantitative or qualitative approach. The quantitative approach focuses on the frequency of specific terms (words, expressions, themes) within a corpus of text, while the qualitative

approach aims to examine lexical choices as well as associations and oppositions between terms, plus the visibility of certain elements in the text (Smith, 2000; Bauer, 2002). In this study, we have opted for a predominantly qualitative analysis because our research question requires the examination of subjective information and a deeper interpretation of the results. As for Atlas.ti, it is a computer-based qualitative data analysis software (CAQD) that streamlines the categorisation of a substantial volume of text - or even audio and visual data - through the use of algorithms. This software replaces the manual coding of texts that is typically employed in the Content Analysis method, thus facilitating the analysis process. The coding process begins with the selection of passages deemed relevant to the research questions, followed by explanations or descriptions of their content for subsequent consultation, comparison, and classification. The data used were collected from proposals related to the oil and gas industry presented in Congress, such as bills, provisional measures, requests, resolutions, legislative decrees, and proposals for amendments to the Constitution. The following proposals with an impact on the oil and gas agenda were found through a preliminary search on the websites of the Chamber of Deputies and the Senate:

 Bill 3924/2012 (incentives for energy production from renewable sources). Bill 3280/2015 (provides for the new National Policy on Climate Change).
 Bill 3834/2015 (requirements for adding biodiesel to diesel).
 Bill 528/2015 (minimum price policy for road cargo transport).
 Bill 6488/2016 (provides for the establishment of both the National Energy Policy Council and the National Agency for Oil)
 Bill 9086/2017 (provides for the National Biofuels Policy, known as RenovaBio). Bill 4476/2020 (promotion of the natural gas industry).
 Bill 3552/2023 (provides for the commercialization of Liquefied Petroleum Gas) Bill 3947/2023 (provides for transparency in the composition of costs and price in the production chain of fuel production)
 Provisional Measure 795/2017 (special regime for oil and gas exploration). Provisional Measure 814/2017 (provides for the generation of thermoelectric energy based on fossil fuels). From that point, we will investigate votes, speeches, and statements made by congressmen in the moment that these proposals were introduced.

Preliminary results: Thematic parliamentary fronts have become increasingly present in the Brazilian legislature since democratisation. These fronts (also known in the literature as congressional member organisations, caucuses, or intergroups) can be defined as an association of congressmen from different parties to promote discussion and legislation on a particular topic (Cascioni and Arajo, 2019; Simionatto and Costa, 2012; Ringe, Victor, and Carman, 2013). These fronts have developed as a result of political parties' compositions, which frequently do not reflect the particular preferences of different societal segments. As a result, supra-party organisations, or so-called informal benches, start to appear in the National Congress with the aim of advancing the causes, ideas, and interests of specific sectors. Although these interests can be diffuse, i.e., related to social problems, moral matters, and environmental and economic concerns, the object par excellence of the parliamentary fronts is directly linked to some type of concrete economic interest from different segments of society (Simionatto and Costa, 2012; Diap, 2022; Vogel, 2005). However, because of their characteristics, non-party fronts are rarely able to determine the votes of their members. Apart from the presentation of the list of signatures for its creation and the statute submitted for its registration, there is no control over participation on Parliamentary fronts. A variety of elements, including regional and corporate affinities, are present within them to varied degrees (Cascioni and Arajo, 2019; Simionatto and Costa, 2012). With regard specifically to parliamentary fronts related to promoting the interests of the oil and gas industry (notably the Parliamentary Front for the Sustainable Development of Oil and Renewable Energy, the Parliamentary Front in Support of Oil, Gas, and Energy, the Parliamentary Front in Defence of Oil Producing Municipalities, and the Parliamentary Front for Natural Resources and Energy), their performance does not seem to have been remarkable, especially when compared to other fronts, especially the well-known Parliamentary Front for Agriculture and Farming. There are several reasons for this. One noteworthy fact is that a large number of oil and gas companies have already increased their efforts to include renewable energy in their portfolio; as a result, they are also very interested in increased government incentives for the production of cleaner energy, leaving the majority of the party and congressional sensitization to the fossil fuel agenda to representatives from regions heavily dependent on these revenues. However, there is still a lot that needs to be clarified about how these legislative fronts operate and whose interests they favour.

Preliminary conclusions: Our initial conclusion is that congressmen aligned with the oil and gas agenda, especially those from constituencies highly dependent on revenues from this industry, have worked to impede initiatives aimed at a rapid transition to cleaner energy by pooling their actions in thematic parliamentary fronts dedicated to protecting the fossil fuel segment. However, the degree of cohesion within these fronts, in addition to the effectiveness and success of their proposals and actions, is still uncertain and needs to be further investigated.

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Abstract Title: CCUS: Legal Developments, Policies and Challenges

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Abstract: Carbon Capture, Utilisation and Storage ("CCUS") has been identified as one of the most advanced technologies available for the reduction of emissions and the reduction of carbon levels in the atmosphere. CCUS is expected to account for almost 15% of the cumulative emissions reduction, and its contribution to the net-zero agenda increases as the technology improves and the related costs fall. Although estimates for the necessary level of growth differ, it is indisputable that a significant expansion of the CCUS technologies is needed to meet Paris Agreement commitments. Expanding CCUS will, however, require governments to address current barriers to the scalable deployment of CCUS techniques. Furthermore, in order to ensure the successful development an deployment of CCUS, legal and regulatory frameworks geared towards ensuring the safety and efficacy must be established. This chapter delves into the legal challenges and concerns with regard to the implementation and use of CCUS, as well as the global trends, legal policies and norms which have emerged. Following this discussion, recommendations are offered towards the mitigation of any barriers against the development and deployment of CCUS. Some of these legal challenges and concerns include the safe and secure storage of CO2, property rights, and disputes as to liability. The approach to CCUS and the global trends, legal policies and norms are explored in the United States, Canada, the United Kingdom and Europe. These States have all utilised their own incentives and policies to encourage the expansion of CCUS technologies across their jurisdictions and have even engaged in international cooperation by implementing bilateral agreements for mutual assistance between States. Notwithstanding, there are still significant barriers to the scalable deployment if CCUS technologies, accordingly, recommendations including CCUS legislation and economic policies have been proffered.

Keywords: key Words: CCUS, Sustainable Development, Legal Framework, United States, Canada, United Kingdom, Europe.

Introduction and Objectives: The deployment of CCUS can help counties reach emissions reductions targets while still pursuing economic growth and a cleaner environment, thus advancing energy justice. Global energy demand is expected to grow between now and 2050 and to outpace the construction of new renewable sources. According to a forecast by the

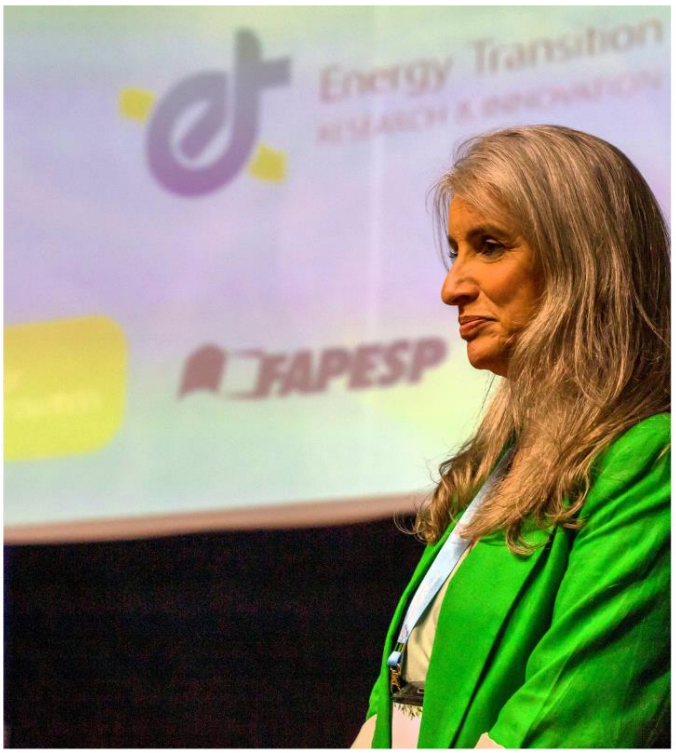
International Energy Agency (IEA), CCUS is expected to account for almost 15% of the cumulative emissions reduction, and its contribution to the net-zero agenda increases as the technology improves and the related costs fall. Similarly, an analysis by McKinsey & Company posits that over 25,000 industrial carbon emitters across the globe can be decarbonised through the adoption of CCUS technologies. Although estimates for the level of growth necessary differ, it is clear that a massive expansion of CCUS is needed to meet Paris agreement commitments.

Expanding CCUS will however require governments to address current barriers to the scalable deployment of CCUS techniques. These include incomplete or absence of regulatory and policy frameworks, lack of emissions reduction mandates such as carbon pricing, insufficient incentives for investment in CCUS technologies, and challenges with social license, justice, and public acceptance of CCUS applications. These barriers inhibit the industrial implementation and up-scaling of CCUS applications. Likewise, the successful development and deployment of CCUS relies on the establishment of legal and regulatory frameworks to ensure the effective stewardship of CCUS activities and the safe and secured storage of carbon. Although regulatory approaches differ, a commitment to scaling CCU necessitates significant public investments in innovation, outreach and education, and regulation. IEA identifies 25 priority legal and regulatory issues for CCUS legislative frameworks including permitting and environmental reviews, enabling first mover projects, addressing liability and transboundary issues, and ensuring safe and secure storage. In addition, legislation should integrate CCUS with other legal frameworks for emissions regulation or reduction, including emissions trading and reporting programs and carbon taxes, and with regulations related to climate disclosures and greenwashing. In some cases, legislative frameworks may also include policies providing specific support to cover for the high costs of CCUS operations. This may include provisions on direct investments in innovation, and research and development, or in loan guarantees, as through the United States programs authorized by the Inflation Reduction Act and the EU's Net Zero Industry Act, or through tax incentives such as those in place in the United States and Canada.

Methodology: Doctrinal Research.

Preliminary results: The achievement of carbon reduction and negative emissions through the adoption of CCUS technology calls for the implementation of appropriate regulations and policies that support the development and deployment of such technology. As affirmed by the United Nations (UN) through its sustainable development agenda, the prevention of climate change requires the integration of preventive and mitigating measures into national policies, strategies and planning. Such regulatory and policy support may take the form of government regulation through the command-and-control approach, market-based regulation and incentives, and the adoption of principles consistent with the just and responsibility deployment of emissions reduction and carbon removal technologies. To meet nationally determined contributions, governments around the world are implementing regulatory and policy support for the development and application of CCUS technology within their jurisdictions.

Preliminary conclusions: Deployment of CCUS is indispensable to the achievement of the climate targets endorsed by the Paris Agreement. Factors such as absence of or incomplete regulatory and policy framework, lack of emissions reduction mandates, insufficient incentives for CCUS investments, etc., however pose significant barriers to the scalable deployment if CCUS technologies. These barriers may be effectively addressed through the adoption of robust legal and regulatory frameworks for CCUS both at national and international levels. Moreover, to ensure sustainable deployment of CCUS, States must enact economic policies to encourage project development, establish and enforce legal frameworks to encourage transparency and protect public interests in health, safety, the environment, and property. Even with appropriate regulatory regimes, CCUS will not achieve its commercial potential without public support. This is required for research and development related to technology demonstration and site characterization. Additionally, to achieve social license and address concerns of distributive justice, deep community engagement, outreach, and education are essential. These efforts are underway to varying extents in jurisdictions worldwide. Communication and knowledge sharing can however help accelerate these developments.


Energy Transition
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Abstract Title: Analysing "O Estado de São Paulo's" perspective on Bioenergy & BECCS

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Abstract: Bioenergy is a sustainable alternative for energy production, standing out for its versatility in raw materials and forms of use. This energy solution has a significant potential to impact climate action, especially when combined with Carbon Capture and Storage (CCS), which is called Bioenergy with
Carbon Capture and Storage (BECCS). It is well known that social perception influences the acceptance and support for energy projects and its investigation is essential to progress in the energy transition agenda. When it comes to the social perception of bioenergy, its range of usage and biomass sources turn out to increase the complexity of this inspection, as there are many different types of bioenergy perception to study, although some similar aspects can be found. This study analysed 171 articles from "O Estado de São Paulo", most from the printed newspaper, the second most read in Brazil. The methodology used quantitative and qualitative analysis through the Atlas TI software. This research aims to find the most prevalent narratives on the bioenergy subject by analysing the social perception of a Brazilian journal that significantly influences the Brazilian population. It is expected that findings will point out that the investigated newspaper is favourable to energy transition using bioenergy, but has its reservations.

Keywords: bioenergy, social perception, energy transition, media.

Introduction and Objectives: As much as energy transition is a central subject to climate change action, the social perception of this theme is crucial to making it possible. Within this context, bioenergy is one of the leading low-carbon solutions for the future, considering its versatility and its low carbon footprint. Using a variety of biomass sources, different products or energy services are obtained from bioenergy production, such as ethanol, biogas, or thermal energy. One of bioenergy's potential relies on the production of biofuels, which can be an important solution for replacing fossil fuels. The biomass production chain itself captures carbon through photosynthesis, but it is also possible to combine Carbon Capture and Storage (CCS) with this alternative, resulting in the so-called BECCS. Those solutions combined play a crucial role in decarbonizing sectors such as heavy industry, aviation, and trucking in the Net Zero Emissions by 2050 Scenario. However, the installation and success of energy projects do

not depend exclusively on industry plans as social perception interferes with its acceptance. We can use as an example the perception of residents living close to biomass power plants or even the society being favourable or not to the clean energy solutions. When it comes to newspapers, their opinion and impressions are fundamental to influencing society's perception of any subject. That being pointed out, this data collection is justified by bioenergy's relevance as a low-carbon solution and by Brazil's noteworthy position in this sector as the world's second-largest producer of biofuels for the transport sector. In this context, the objective of our work is to research and interpret the social perception of bioenergy using Social Sciences such as Social Psychology to understand society's views and sentiments towards bioenergy and use this knowledge to impulse the carbon neutrality agenda.

Methodology: To investigate the most prevalent narratives and discussions on bioenergy and BECCS, this study uses published articles of the mass circulation Brazilian newspaper "O Estado de São Paulo", that is almost 150-year-old and a traditional Brazilian newspaper that has a significant influence on national media, being the second-most printed paper in the country and one of the most read in Brazil's business capital. By selecting this newspaper to be our analysed data, our study aims to investigate the narratives that influence millions of Brazilians every day. To select the articles, the word "bioenergy" and "BECCS" was filtered using the search tool from the newspaper's website, limiting the period from January 2018 to July 2023. It was used as criteria to target all the published articles from Jan 2018 to August 2023, considering the increase of the international interest on the climate acting theme in the last years. A copy of these articles was transferred to ATLAS.ti to initiate the analysis. ATLAS.ti. is a computer assisted qualitative data analysis software that facilitates analysis of qualitative data for qualitative research, quantitative research, and mixed methods research. This tool that supports locating, coding/tagging, and annotating features within bodies of unstructured data. By choosing this software, our investigation aims to frame a content analysis of "O Estado de São Paulo's" most prevalent opinions on bioenergy and BECCS.

Preliminary results: This study aims to analyse and contribute to understanding the narratives and feelings of a relevant Brazilian press media vehicle. Our investigation contributes to comprehending society's perception of bioenergy and BECCS, which has great importance to the government and to companies interested in investing in those solutions. To generate valuable data for those objectives, this investigation aims to present specific period-related narratives and numbers, connected to important national and global events. On this matter, it is expected to discover a higher frequency of publications close to global environments such as COPs and other United Nations events, and to find an increase in publications on bioenergy and BECCS over the years. Also, our study expects to classify and analyse the most prevalent feelings in the investigated publications, having in prospect to find favourable feelings about companies' investments in clean energy and mixed feelings about the Brazilian government's position in this matter. When publishing energy transition-related articles, "O Estado de São Paulo" allocates the subject to the Economy & Governance category, indicating a potential tendency to share a business-influenced perspective. Therefore, is expected to find frequent

Environment, Social and Governance (ESG) and company-related news, promoting a positive and hopeful view on investing in bioenergy projects.

Preliminary conclusions: Brazil has a historical-constructed relationship with biofuels, which contributes to the society's knowledge and proximity to this solution - which we cannot extend to BECCS. Furthermore, Brazil has great bioenergy potential, maintaining this solution as one of the most reliable from the perspective of society in the country. Considering these points, it is possible to understand that there is a tendency to find positive perspectives regarding the advancement of bioenergy in the country. Other advances have been made in the country in this regard, such as the development of hydrogen fuel from ethanol, proving to be a solution that generates even more clean energy options. Therefore, it is important to be informed and delve deeper into the perceptions of Brazilian society about this solution.

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Abstract Title: Decarbonisation in the view of Brazilian Media and Parliament: Impact on Public Perception and Consequences for Energy Transition Projects – **SRS205**

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Abstract: The aim of this study is to assess how the idea of decarbonisation and the energy transition by the oil & gas industry has been approached by Brazilian stakeholders, especially by media outlets and political actors. To do this, we will analyse articles on the subject from the newspapers with the highest print circulation in Brazil, as well as statements and legislative proposals made by political actors. This comprehensive analysis encompasses the period spanning from 2013 to 2023. After identifying the main ideas from these stakeholders, we will deepen the analysis through in-depth interviews using a quantitative and qualitative Q-methodology analysis. Our hypothesis is that the way these actors perceive and communicate the issue of decarbonisation plays a fundamental role in the alternatives proposed for emissions reduction and energy transition in the country. Additionally, their views as opinion leaders have

a significant influence on public perception towards or against alternatives and players. Therefore, we aim to identify which alternatives they envisage when the issue of decarbonisation is raised and whether these alternatives materialise in legislative proposals to the parliament. Finally, we aim to map narratives and sentiments - positive, negative, or neutral - about the oil & gas industry's decarbonisation process and energy transition efforts.

Keywords: Brazilian Media, Brazilian Parliament, Oil & Gas, Decarbonization, Energy Transition, Public Perception, Grounded Theory, Q-Methodology.

Introduction and Objectives: Public perception of decarbonisation is of fundamental importance to energy transition projects. Public resistance can be one of the greatest challenges to the implementation of these projects since the reproduction of certain discourses, either by the media or by politicians, provides the general public with tools with which a problem is constructed, dominating the way a given society thinks about it (Hajer, 1995).

Therefore, this study aims to monitor social perceptions about decarbonisation in the oil & gas industry in Brazilian society, investigating how certain discourses and narratives shape perceptions and attitudes about the subject. By examining different media coverage, we seek to identify how the energy transition is portrayed in these discourses and what alternatives (i.e., renewable energy, cutting-edge mitigation technologies, energy efficiency) are offered. By examining proposals and statements made in the Brazilian parliament, we aim to analyse the media impact on the political arena as well as the alternatives envisaged by Congressmen. Finally, we will examine which narratives actually end up in legislative proposals.

A further step is to assess how these discourses are, in fact, assimilated by some key actors (academics, business people, politicians, influencers). This assessment will be made using the Q methodology. The final objective is to create an analytical framework that identifies the dominant narrative lines regarding the energy transition in Brazil, classifies certain categories of thinking, and proposes hypotheses for subsequent research.

Methodology: Our methodological framework consists of (i) Grounded Theory, supported by the Atlas.ti software; (ii) interviews using the Q Methodology.

The choice of Grounded Theory stems from the fact that this study is exploratory in nature. It departs from the elements brought by the texts to propose categories of analysis rather than conforming the data to a specific theory. According to Denscombe (2007), grounded theory analysis seeks to identify key concepts through the use of codes and categories. The development of these concepts is the main purpose of the analysis, as they offer a new perspective on the data and form the basis for any theories or broad generalisations that may emerge from the study.

A computer-aided qualitative data analysis (CAQD) programme called Atlas.ti will help to

categorise the texts through the use of algorithms. This programme speeds up the analysis process by replacing the manual coding of texts. The coding process consists roughly of selecting passages of text that may be relevant to the study, followed by a description or explanation of their content for later consultation, comparison, and classification.

The data used was collected from four Brazilian newspapers (Folha de São Paulo, O Globo, Estado de São Paulo, and Valor). These four outlets were chosen because they are the four largest in terms of digital subscriptions in Brazil (Reuters, 2023; Yahya, 2023; Lubianco, 2021). Regarding the parliament, we collected proposals related to the oil and gas industry presented in Congress, such as bills, provisional measures, resolutions, and legislative decrees, as well as statements made by congressmen, especially those that are part of parliamentary fronts related to the interests of the oil and gas industry.

The second step of the research will be to apply the Q methodology to key stakeholders. The interviews will be used to gain a better understanding of how they understand concepts such as decarbonisation and energy transition and what alternatives they see on the horizon. The Q approach was adopted in order to extract latent discourses from the data provided by the stakeholders by aggregating and correlating individual responses (Barry & Proops, 1999).

Results: With regard to the public opinion issued by the Brazilian media, our initial hypothesis is that the media discourse of the analysed media outlets does not differ significantly from each other, with the issue of decarbonisation and the energy transition being dealt with depthlessness. So far, we have noted a tendency for more reports during events such as climate summits or extreme weather episodes. We have also noted a tendency to reproduce discourses that come from the international media, some of which are not always applicable to the Brazilian reality and are therefore replicated in an uncritical manner. Another way in which the subject is exposed in the media is through content sponsored by companies or institutions.

The issue of energy generation - especially with regard to fossil fuels - is portrayed around the world through discourses and narratives not always accurate in the particularities, simplifying complex issues. Therefore, the uncritical reproduction of certain discourses competes to hinder possible alternatives, which can differ considering each country’s resources and potentialities.

In the political sphere, it is expected that parliamentarians with constituencies in states where the oil and gas industry plays a fundamental role in the economy (e.g. Rio de Janeiro) will have their agendas more closely tied to the industry's interests and will move away from the discourse of rapid energy transition, emphasising the importance of the oil and gas sector in generating income, jobs and energy security. We, therefore, expect their behaviour in Congress to follow this agenda, either with a nationalist/developmental stance (e.g. in favour of state participation and Petrobras) or with a liberal approach (e.g. in favour of privatisation and involvement of the

major oil companies).

We believe that the narratives coming from media and political actors have a strong influence on the understanding of other stakeholders involved in energy transition, from experts to lay public, which needs to be confirmed by the Q methodology.

Preliminary conclusions: Our preliminary conclusion is that the way in which the issue of decarbonisation is communicated by the country's key opinion makers is crucial to society's understanding of the problem and therefore plays a crucial role in the selection of mitigation projects. We believe there is a strong correlation between how the media and politicians portray certain mitigation alternatives and the adoption of legislation to make them feasible. In addition, we believe they also influence the perceptions of key stakeholders on the issue and society in general.

0811 - BECCUS3 (TV2)

Chairs: Hamilton Varela – Marcos Buckeridge

Andrieza de Aquino Eslabão
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Abstract: Brazilian Regulation On BECCS: Aps, References and Relevance

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Abstract: Carbon removal technologies (CDR) appear in most of the scenarios outlined by the IPCC for the achievement of the objectives outlined by the Paris Agreement. Among them, the technology that combines bioenergy production associated with carbon capture and storage (BECCS) stands out for its double absorption of CO2, either in the biomass production phase or in the use of the capture method. Several studies show that Brazil has significant potential for the use of BECCS technology to reduce its emissions and comply with international agreements. The present study aimed to analyze the Brazilian regulation on the subject and compare it with international standards. To do so, the methodology used was legislative and bibliographical descriptive and explanatory research, based on the legal method of deductive and comparative reasoning. It was possible to identify that Brazil does not have a specific regulation for BECCS, being, however, applicable by analogy to other regulations, such as the National Policy for Climate Change, the National Solid Waste Policy, the National Policy for

Biofuels and the Bill No. 1425 of 2022, which aims to regulate the capture and storage of carbon in the country. In addition, some points of convergence were detected between the aptitude and pertinence of the Low Carbon Fuel Standard adopted by the State of California, in the United States, which could, once again, positively inspire Brazilian legislation in the sense of encouraging the expansion of technology to take advantage of the national potential in the ethanol industry.

Keywords: Bioenergy. BECSS. Negative emissions.

Introduction and Objectives: The latest report prepared by Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC, 2021) offers relevant new scientific evidence that makes it unequivocal that the global climate system is changing under the influence of human activities, resulting in losses that influence the global ecosystem.

Pörtner (2022), referring to the report, points out that "any delay in global, coordinated and joint action will lead to the loss of a brief window, which is rapidly closing, to ensure a habitable future" and that global efforts to take effective action to mitigate greenhouse gas emissions have so far not had the necessary effects. The results of integrated assessment models show that the energy transition will require more than rapid mitigation of greenhouse gas emissions but also technologies for removing GHGs from the atmosphere, the so-called CDRs (carbon dioxide removal) to achieve a life cycle of a given activity with capture than emissions (negative emissions) (IPCC, 2019). In this sense, technologies that integrate existing activities and adapt them to mitigate or reduce greenhouse gas emissions, aggregating them to generate other social benefits, have great potential to contribute to the country's goals. Most of the scenarios outlined by the IPCC that approach the limit of 1.5°C above pre-industrial temperatures consider the use of technologies that directly or indirectly result in negative carbon emissions, or NETs (IPCC, 2022). Bioenergy production technology with carbon capture and storage (BECCS) combines the generation of energy (electricity or fuel) associated with the capture of GHGs throughout its life cycle and the consequent storage of carbon dioxide permanently (IEA, 2022). According to recent literature, the bioethanol production industry has the potential to develop this technology (Tanzer et al., 2021). However, studies indicate that BECCS technology is unlikely to grow without a supportive regulatory framework and political attention (Fridahl; Lehtveer, 2018).

In this context, this article sets out to investigate i) whether there is Brazilian legislation on BECCS ii) which national legislation can be applied to BECCS by analogy in the event of a legal gap iii) and which international legislation can inspire a potential national framework on this technology. IPCC, 2022: Climate Change 2022: Impacts, Adaptation and Vulnerability. Contribution of Working Group II to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [H.-O. Pörtner, D.C. Roberts, M. Tignor, E.S. Poloczanska, K. Mintenbeck, A. Alegría, M. Craig, S. Langsdorf, S. Löschke, V. möller, a. okem, b. rama (eds.)]. Cambridge University Press. Cambridge University Press, Cambridge, UK and New York, NY, USA, 3056 pp., doi:10.1017/9781009325844.

Methodology: The methodology applied is based on descriptive and explanatory legislative and bibliographical research using the legal method of deductive and comparative reasoning,

whose methodological cut was based on the framework of federal laws and those of selected countries.

In order to research the relevant national regulations on the subject, consults in the Brazilian websites of the Planalto Federal and the Senado Federal was made. The analysis of the selected regulations focused on what they say about the use of biomass energy and the reduction of greenhouse gas emissions, seeking to identify the extent to which BECCS technology fits into the guidelines. In order to search for international regulatory references, the first step in the research methodology used was to identify the countries that already have BECCS projects in operation using the Global CCS Institute database. So Scientific articles were then searched for in the multidisciplinary databases Scopus and ScienceDirect, using the terms: "regulation and BECCS"; "legislation and bioenergy and carbon capture" and "regulation and bioCCS".

In addition to the search for scientific articles, official websites of the state and national governments of the countries where commercial BECCS projects were located were consulted to access the policies that promote the technology. Pörtner, Hans-Otto., IPCC. Sixth Assessment Report: Impacts, Adaptation and Vulnerability. Press Release. P28 Feb. 2022. https://www.ipcc.ch/report/ar6/wg2/resources/press/press-release/. Acess: 29 aug. 2023. IPCC, 2019: Summary for Policymakers. In: Climate Change and Land: an IPCC special report on climate change, desertification, land degradation, sustainable land management, food security, and greenhouse gas fluxes in terrestrial ecosystems [P.R. Shukla, J. Skea, E. Calvo Buendia, V. Masson-Delmotte, H.- O. Pörtner, D. C. Roberts, P. Zhai, R. Slade, S. Connors, R. van Diemen, M. Ferrat, E. Haughey, S. Luz, S. Neogi, M. Pathak, J. Petzold, J. Portugal Pereira, P. Vyas, E. Huntley, K. Kissick, M. Belkacemi, J. Malley, (eds.)]. https://doi.org/10.1017/9781009157988.001

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https://www.iea.org/reports/bioenergy-with-carbon-capture-and-storage, License: CC BY 4.0 Tanzer, S. E., Blok, K., & Ramírez, A. (2021). Decarbonising Industry via BECCS: Promising Sectors, Challenges, and Techno-economic Limits of Negative Emissions. In Current Sustainable/Renewable Energy Reports (Vol. 8, Issue 4, pp. 253–262). Springer Nature. https://doi.org/10.1007/s40518-021- 00195-3

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Preliminary results: Even though there are ongoing projects and research indicates an untapped potential regarding BECCS technology, national legislation has not been developed with it as a focus or designing all possible uses for its expansion in the country. It can be inferred that there are still regulatory gaps and room for policies and mechanisms that can provide security for the expansion of the sector and take advantage of the potential to contribute to the

international obligations to reduce greenhouse gas emissions. Even though there are still no specific regulations in Brazil, can't be said that it is unfeasible to set up a BECCS project in the country since various regulations can be used analogously for its implementation. Law No. 12.187 (National Climate Change Policy), of December 29, 2009, Law No. 12.305 (National Solid Waste Policy), of August 2, 2010 Law No. 13. 576 (National Biofuels Policy), of December 26, 2017, and potentially Bill 1425, of 2022, added to the environmental licensing procedure, would already be enough to support energy use measures linked to BECCS and measures to reduce greenhouse gas emissions in all sectors considered difficult to decarbonize. According to its justification, the project aims to fill a regulatory gap, creating legal stability that allows the agents involved some security for long-term investments. Brazil's potential for combining the production of bioenergy with CCS (BECCS) is also highlighted in the justification, which mentions it as a first step on a disruptive path of no return for a country at the forefront of environmental issues to become more competitive in offering products with "negative emissions" (Prates, 2022).

As in Brazil, most of the countries studied do not have specific regulations for BECCS technology, basing it on various federal or state guidelines, such as those regulating access to land, atmospheric emissions, access to geological sinks and carbon capture and storage (CCS) technology. A search of the Global CCS Institute database (https://co2re.co/FacilityData, 2023) revealed that BECCS projects exist in the following countries, in addition to Brazil: The United States, Sweden, Canada and the United Kingdom.

Considered the "most progressive specific incentive globally" the US Section 45Q tax credit for carbon sequestration denotes the maturity of the Country's regulations to open up a huge market (GLOBAL CCS INSTITUTE, 2021).

At the state level, the most relevant program to mention is the one implemented by the State of California called the California Low Carbon Fuel Standard (LCFS). The project is part of a broader set of programs in California to reduce greenhouse gas emissions (California, S/D).

The LCFS is designed to encourage the use and production of low-carbon fuels in the transportation sector and therefore reduce GHG emissions and decrease the sector's dependence on oil (California, S/D). The policy has already been associated with RenovaBio is the Low-Carbon Fuel Standard.

Preliminary conclusions: This study set out to analyse Brazilian regulations on bioenergy technology combined with carbon capture and storage (BECCS), seeking to identify gaps, find references and highlight the importance of the technology in the current climate change context, where it is necessary to reduce greenhouse gas emissions. In order to do this, it started with some research questions, from which it was possible to identify that Brazil does not have specific regulations for BECCS, although it is possible to apply other regulations by analogy, such as the National Climate Change Policy; the National Solid Waste Policy; the National Biofuels Policy and Bill 1425 of 2022, which aims to regulate carbon capture and storage in the country. It was also possible, through a comparative study of other countries' regulations on the subject, to identify some points of convergence between the potential and relevance of the Low-Carbon Fuel Standard policy adopted by the State of California in the United States of America,

which could positively inspire Brazilian legislation in order to encourage the expansion of technology to take advantage of the national potential in the ethanol industry.
Adopting another calculation model more geared towards the expansion of BECCS technology could make it more attractive, insofar as it could represent a negative emission in a global market. The conclusion is that it is important to have specific regulations coordinated with planning and stimulus policies, considering the particularities and the national context. Brasil. Lei nº. 12.187, de 29 de dezembro de 2009. Política Nacional para as Mudanças Climáticas – PNMC. Brasília: DOU 30.12.2009. https://www.planalto.gov.br/ccivil_03/_ato2007-2010/2009/lei/l12187.htm
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Abstract Title: Hormonal signaling network can contribute to design strategies to improve sugarcane growth and yield

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Abstract: Sugarcane is an essential crop in the Brazilian agricultural scenario, mainly used as a feedstock for sugar and bioethanol production, contributing to mitigate carbon emissions. Attention to the production of biofuels has led to a scientific advance in understanding sugarcane physiology, biochemistry, and molecular biology. Integrating the sugar sensing and signalling processes with hormonal networks systemically helps design strategies to modulate plant growth, increase yield, and adapt to different climatic conditions. Here, we employed biochemical analyses to determine the levels of polyamines (PAs), amino acids, abscisic acid (ABA), and indole-3-acetic acid (IAA) in leaves and culms of sugarcane. Also, a bioinformatic analysis was performed to identify a set of genes related to these biosynthesis and hormonal signalling pathways. PAs were most abundant in leaves, particularly putrescine. The most abundant amino acids were ornithine and lysine in leaves and asparagine, glutamine, and histidine in culms. High levels of hormones IAA and ABA were detected in leaves during the last month of sugarcane development. A deep search by genes related to receptors and signalling of ABA, BR signalling, PAs-, ethylene- and amino acids-biosynthesis allowed the recovery of 3042 sequences from 7 sugarcane databases (transcriptomes and genomes). After restrictive filtering (coverage, presence of domains, and removing redundant sequences), 784 candidate sequences remained corresponding to 36 groups of genes from the pathways described above. In silico expression profiles revealed that genes related to PAs biosynthesis and ABA- and BR-signalling were the most expressed in two sugarcane transcriptome datasets (root development and stress conditions). These findings could be used to genetically modify

sugarcane to accelerate growth and sugar accumulation.

Keywords: hormones signalling, growth, carbon, bioenergy, metabolism.

Introduction and Objectives: Integrating the sugar sensing and signalling processes with hormonal networks constitutes a strategy to increase the capacity and resilience of crops to extreme environmental conditions. In this way, is fundamental to understand the plant hormones signalling pathways through studies that promote a better knowledge of stress responses, cell wall structure, and energetic metabolism. The integrative plant perception and management of carbohydrates and other metabolites could serve as a control mechanism to integrate external environmental factors, nutrient homeostasis, developmental programs, and stress response to anabolic and catabolic processes. In this core, amino acids and plant hormones pathways [including polyamines (PAs), brassinosteroids (BRs), abscisic acid (ABA), auxins as Indole-3-acetic acid (IAA)], as well receptors and signalling components act in concert in numerous plant physiological processes, which determine the cell fate and differentiation, tissue and organ development, or environment responses.

This complex network can lead to the breeding of important crops used as sources of food or bioenergy, such as sugarcane. Sugarcane is an important crop in Brazilian agriculture and bioenergy scenarios and a broader physiological and molecular coverage can aid in understanding its metabolism, helping to elucidate the metabolic pathways that influence crop gain of yield.

Here, the identification and characterization of the biochemical and molecular variation in the hormonal signaling components in sugarcane is reported. This study includes plant hormone and amino acid profiles in a sugarcane growing in the field during 12 months, and the identification of a set of genes expressed in sugarcane under different conditions. For this, two strategies were employed: i) a biochemical profile during sugarcane development in the field, and ii) identification and characterization of genes related to receptors and signaling of ABA, BR signaling, PAs-, ethylene- and amino acids biosynthesis, in two sugarcane transcriptome datasets.

Methodology: Plant material:

Green fully expanded leaves and culm from sugarcane plants grown in the field were collected in 01, 03, 06, and 12 months of development, according to De Souza et al. (2018). The plant material was ground in liquid nitrogen and used for biochemical characterization.

Biochemical analysis:

Putrescine, spermidine, and spermine were extracted according to de Oliveira et al. (2018). Samples were homogenized with cold 5% of perchloric acid and subjected to three cycles of freezing and thawing. After centrifugation, the supernatants containing the free PAs were collected and derivatized. Dansylated PAs were extracted with 200 µl of toluene and the supernatant was collected and dried under nitrogen. Dansylated PAs were dissolved in 200 µl

of acetonitrile.

The extraction and determination of free amino acids were performed according to de Oliveira et al. (2018). Aliquots of fresh material were extracted with 80% ethanol. Amino acid derivatization was realized with o-phthalaldehyde.

The hormones ABA and IAA were extracted and quantified according to Álvarez-Florez et al. (2017) and Silveira et al. (2008), with modifications. Fifty mg of the dry weight of leaves and culms were homogenized in 2.5 ml extraction buffer containing methanol and isopropanol (20:80), 1% acetic acid, and 0.5 µCi.ml-1 of [3H]IAA and [3H]ABA (internal standards).

The metabolites were separated by HPLC on a reversed-phase C18 column (5 µm x 4.6 mm x 250 mm). PAs were detected at 340 nm (excitation) and 510 nm (emission) wavelengths with a RF-20A fluorescence detector. ABA content was determined using a UV-VIS detector at 254 nm, while IAA content was determined using a fluorescence detector at 280 nm (excitation) and 350 nm (emission).

Bioinformatic analysis:

A bioinformatic approach was employed to identify a gene set related to PAs-, ethylene- and amino acids-biosynthesis, and ABA and BR signalling pathways. The main genes comprising these networks (receptors, transcription factors, and enzymes) were first identified and characterized in model species (Arabidopsis, rice, and maize), through Tair, Phytozome, Rice Genome Annotation, and Maize Genomics Resource platforms. These sequences were used as queries to identify and recover sequences from seven sugarcane databases (transcriptomes and genomes). Restrictive filtering including coverage and presence of domains, as well as the removal of redundant sequences, were employed to maintain those reliable sequences with high identity. Sequences were grouped through EGGNOG code related to domains annotated in the EGGNOG platform.

In silico expression analysis (CPM values) were performed by using two sugarcane transcriptome datasets: i) from four segments of roots, during aerenchyma development; and ii) from sugarcane plants growing under stress conditions (control, drought, elevated CO2, or by a combination of them). A heatmap and Hierarchical cluster by Euclidean distance was performed using the CPM expression values.

Preliminary results: PAs, amino acids, and hormonal profiles in sugarcane field

In all months analysed, PAs were most abundant in leaves. The content of each PA in the leaf and culm revealed that the highest amount in the total PAs during month 01 was caused by putrescine and spermidine, respectively. Putrescine was the main PA in the leaf along the sugarcane development, followed by spermidine and spermine. During the sugarcane development, the amino acid content was more constant in the leaf than in the culm, in which the total amino acid levels were 12 times higher in the month 01. The most abundant amino acids found in the leaves were ornithine and lysine, whereas in culm were asparagine, glutamine, and histidine.

Sugarcane leaf and culm have different IAA and ABA profiles during development, especially

concerning IAA abundance, which was much higher in the leaf at most time points analysed.

High levels of hormones IAA and ABA were detected in leaves during the last month of sugarcane development. In silico mining of hormonal signalling network in sugarcane A deep search by genes related to receptors and signalling of ABA, BR signalling, PAs-, ethylene- and amino acids-biosynthesis, allowed recovery of 3042 sequences from 7 sugarcane databases. This amount is 18, 23, and 25 times more than found in Zea mays (170 sequences), Oryza sativa (132 sequences), and A. thaliana (120 sequences), respectively. After restrictive filtering, 784 candidate sequences remained corresponding to 36 groups of genes from the pathways described above. A search on two sugarcane transcriptome datasets realized by Lafieco's group was performed to recover both sequence and expression values (CPM). In the root transcriptome dataset, 454 sequences were expressed in the four root segments, and 240 were differentially expressed (DEG) among the segments. In leaves from sugarcane growing under different stress conditions, 260 sequences were expressed, and 65 were DEGs. PA biosynthesis/catabolism pathways and members related to the SnRK2 subfamily were the pathways with the greatest number of genes.
In silico expression profiles revealed the pattern of the primary genes expressed in this hormonal signaling network. In root transcriptome, genes related to PAs biosynthesis and catabolism (SAMS, SAMDC, SPDS/SPMS, ALDH, and CuAO), SnRK2, and ABA- e BR-signaling genes were the most expressed genes in all root segments. Ethylene biosynthesis genes (ACS and ACO) are low expressed, suggesting that methionine is directed to PA biosynthesis during the root development. In the sugarcane stress experiment, genes related to spermidine and spermine biosynthesis (SAMS, SAMDC, SPDS/SPMS) are slightly more expressed under elevated CO2 conditions. Most genes involved in ethylene biosynthesis genes are low expressed under these conditions. Genes related to ABA signaling (PP2C-A) and proline biosynthesis (P5CS1/2) showed high expression values, indicating their participation in the stress response.

Preliminary conclusions: In summary, this study allowed a detailed analysis of hormonal signalling network components in sugarcane plants by two strategies: i) a biochemical profile during sugarcane development in the field, and ii) through identification and characterization of genes related to receptors and signalling of ABA, BR signalling, PAs-, ethylene- and amino acids-biosynthesis, in two sugarcane transcriptome datasets. In the first strategy, biochemical analyses revealed different profiles between the two organs analysed (leaves and culm), and also during the sugarcane development in the field. These changes provide insights into distinct metabolic profiles of each organ throughout development and pave the way for a more integrative understanding of the biological functioning of sugarcane in the field, which can contribute to future strategies to improve yield performance. In the second strategy, the main set of genes involved in hormonal signalling in sugarcane was identified. Differentially expressed genes were observed in each transcriptome dataset analysed, demonstrating variations among PAs biosynthesis and catabolism, and ABA- and BR-signalling. These differentiated responses to stresses will be assessed by physiological measurements (hormonal,

amino acids, carbohydrates, and biomass profiles) in sugarcane overexpressing the gene RAV (RELATED TO ABI3/VP1), which is induced by a balance between auxin and ethylene, and lead to a repression effect on the EPG1 (ENDOPOLIGACTURONASE1), involved in the expression of pectinases genes. This study allows a detailed analysis of the partial core hormonal signalling components in sugarcane and these findings provided suitable targets for genetic engineering in sugarcane to accelerate growth and sugar accumulation.

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Abstract Title: Electrochemical conversion of CO2 into oxalate with negative carbon footprint

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Abstract: Considering the approaches of CO2 conversion, the electrochemical methods have received increasingly attention. It is possible to use renewable energy to produce high added-value products from CO2 industrial emissions, resulting in carbon neutral footprints. Preliminary techno-economic analysis of an electrochemical reactor for CO2 conversion, showed that oxalic acid has a great potential to achieve negative carbon footprints. In this study, we show the initial experimental obtained in our first reactor prototype, where Faradaic efficiencies of 60% are already achieved.

Keywords: CO2 reduction; oxalic acid; electroreduction.

Introduction and Objectives: The electroreduction of CO2 into oxalic acid/oxalate is a challenging process in terms of applicability. Firstly, the formation of the intermediate state CO•- demands high energy prior to form oxalate ion. Secondly, a variety of products can be formed according to the electrocatalyst and the solvent chosen, thus the selectivity is an essential factor for the efficiency of the system. Most of the publish studies aim to develop new catalyst materials which, although very important, is not the only challenge to be overcome. The system efficiency is also related to the reactor type, its specific design and operating conditions. Currently, it is well-known that the conversion of CO2 into oxalate ion can only occur using aprotic media. Also, lead is considered the best electrocatalyst for this reaction, presenting high selectivity. Although not ideally feasible, these factors are a great starting point for the development of a new electrochemical reactor. Thus, our main objective is to produce oxalic acid with negative carbon footprint in a novel device for CO2 electroreduction.

Methodology: Experiments were carried out in a membraneless electrochemical reactor (produced by additive manufacturing) connected to a flow system with recirculation. Electrodes were two plates (10 mm²) of stainless steel and zinc as cathode and anode, respectively, maintained in a 2 mm distance. Electrolysis was carried out in a PAR potentiostat during 2 h. The working solution – acetonitrile with tetrabutylammonium perchlorate – was saturated with Ar for 20 min followed by CO2 for 30 min prior to each experiment. After the electrolysis, the solution was filtered, and the solid oxalate was dissolved in H2SO4 (3M) to be analysed by HPLC.

Preliminary results: Previous tech-economic analysis showed how efficient an electrochemical reactor must be for a viable carbon abatement pathway. It was found that, among the major CO2 reduction products, oxalic acid has the greatest potential to achieve negative carbon footprints (followed by formic acid, CO and ethylene). Considering the Brazilian energy matrix, oxalic acid production leads to a negative carbon footprint for an electrochemical reactor operating with conversion efficiency higher than 20%. Meanwhile, for an energy matrix similar to USA, the reactor would have to operate above 50% conversion efficiency to achieve the same result. In this context, we developed a new electrochemical device focusing on the conversion of CO2 into oxalic acid. The first prototype was tested under different applied currents (10 – 70 mA/cm²), flow rates (10 – 50 mL/min) and concentrations of supporting electrolyte (0.025 – 0.1 mol/L). At 30 mA/cm² it was possible to achieve a faradaic efficiency (FE) of 60%, which corresponds to a production of 0.3 mg/h.mm² with the lowest energy consumption (EC) of 46 W.h.L/g. Higher current densities also showed a maximum FE of 60% but resulted in higher costs due to the energy consumption. As expected, for laminar flow, the higher the fluid velocity the higher the FE. Similarly, the lower the concentration of supporting electrolyte, the lower the FE. Although these results are expected, it is important to evaluate each operational parameter to further optimize fine details of the reactor design. These initial results already show efficiencies as good as the found in the literature, however with a much lower cost.

Preliminary conclusions: Our first reactor prototype already showed 60% efficiency for the conversion of CO2 into oxalic acid. This result is highly competitive with the literature findings, especially regarding reactor and process costs.

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Abstract Title: Fingerprinting agro-industrial wastes: a promise for biomaterials

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Abstract: Population growth and climate change demand an increase in the use of land, food, and energy, which requires sustainable development to ensure health and well-being for society. To achieve sustainability, employing different feedstocks into value liquid fuels and value-added bioproducts is essential. The cell wall is the largest terrestrial carbon source and can be used for bioenergy. This structure is composed of a cellulose core in which lignin and hemicelluloses are crosslinked to it, and immersed in a pectin matrix that forms a different polysaccharides architecture in species and tissues. The characterization of different agro-industrial wastes allows the study of these biomasses in the circular economy and is aims for this work. We characterized 19 different biomasses and evaluated their potential as a by product and in bioenergy. The cell wall of the biomasses was fractionated as pectins, pectins+soluble hemicelluloses, and cellulose by physical-chemical treatments. Its weight balance was estimated, and the monosaccharide´s fractions composition was obtained after acid hydrolysis. The feedstocks corn cob, corn straw, soybean husk, and industry paper residue had higher saccharification capacity despite their low content of lignin and uronic acids, and cell wall composition of 30% glucose and 60% xylose. Therefore, those feedstocks, along with sugarcane, are more promising for bioethanol production, while duckweed, barley, sorghum, wheat, rice, bean, and coffee residues could be used for other by-products in green chemistry for the generation of value-added products.

Keywords: feedstock, residue, cell wall, polysaccharides, and carbohydrates.

Introduction and Objectives: Population growth is estimated to reach 9 billion people by 2050 (HLPE, 2017). This growth, along with climate change, demands an increase in land, food, and energy use, which requires sustainable development to ensure health and well-being for society. To achieve sustainability, employing different feedstock into valuable liquid biofuels and other value-added bioproducts is essential (Mishra et al., 2020). The major available feedstock is biomass, where plants fixate carbon through photosynthesis, mainly in cell wall polysaccharides (Verbančič et al., 2017). The cell wall is a rigid and complex structure of pectins, hemicellulose, cellulose, lignin, and proteins surrounding each plant cell. This structure is organized in a cellulose core in which hemicellulose and lignin are strongly attached and crosslinked, immersed in a pectin matrix (Carpita & Gibeaut, 1993). The primary cell wall is expansive, constitutes 90% of its dry weight as polysaccharides, and is classified as types regarding its domains (pectins, hemicelluloses, and cellulose) proportion and main hemicellulose (Carpita & Gibeaut, 1993). Cell walls are known to have distinguished architecture and chemical composition between species and organs (Carpita & Gibeaut, 1993; de Souza et al., 2013). The organization of the polysaccharides has distinct linkages according to the chemical composition of the plant, and those composition and interaction between the polymers could be as a map for possible applications. Therefore, it is important to characterize and elucidate the chemical structure of several cell wall models from distinct biomasses by biochemical and genetic analysis (Sarkar et al., 2009).
Despite the biomasses diversity, agro-industrial wastes are grouped as wood product industries wastes, municipal solid waste, agricultural residues, and dedicated energy crops (Saini et al., 2015). In the world, 181.5 billion tons of lignocellulosic biomass are produced yearly (Ashokkumar et al., 2022). Of these, 4.6 million tons are agricultural wastes, but only 1.2 billion tons have further applications (Dahmen et al., 2019). A large part of the crop's biomass (husks, seeds, roots, bagasse, molasses, leaves, stems, straws, and bark) is not used. Therefore, it is a great feedstock that can be employed for the generation of biotechnological products (Arpit Singh et al., 2022). Thus, the present work aimed to characterize 19 agro-waste and evaluate their potential as by-products of biomaterials. Depending on the composition of the agro-waste, the calorific power varies, as well as the cell wall polysaccharide hydrolysis, which could be improved with different cocktails.

Methodology: ineteen agro-wastes were obtained and analyzed in the cell wall composition. Sugarcane, energy cane V2, energy cane V3, sugarcane bagasse from industry, barley bagasse, sorghum residue, corn cob, corn straw, wheat bran, rice husk, soybean straw, soybean residues (leaves +stalk), soybean husk, coffee husk, bean straw, duckweed, pruning tree residue, eucalyptus chip, and industry paper residue (pulp and paper milled sludge) residues were dried at 50 °C and grounded in ball-mill. The agro-wastes were analyzed towards the lignin (acetyl bromide method) (Fukushima et al., 2015; Fukushima & Kerley, 2011)., uronic acid content (Filisetti-Cozzi & Carpita (1991), saccharification, and cell wall composition. Cell wall

polymers were isolated by the physical-chemical treatments of the fractionation (Gorshkova et al., 1996), and the composition monosaccharides composition of the pectins, hemicellulose, and cellulose was determined by an acid hydrolysis quantified in HPAE-PAD. For the fractionation process, the agro-wates were extracted exhaustively with 80% ethanol at 80 °C for 20 min each. The residue was recovered by centrifugation, dried, and the starch was extracted with DMSO 90%. The de-starched AIR (cell wall) was extracted 0.5% ammonium oxalate (pH 7.0) for pectin solubilization. The ammonium oxalate residues were extracted with sodium chloride 3% (m/v) in acetic acid 0.4% (v/v) for lignin removal and acquisition of pectin + soluble hemicelluloses. The sodium chlorite residues were extracted with 4M NaOH with 3 mg.mL-1 sodium borohydride to solubilize the hemicelluloses. And the obtained residue was mainly cellulose. After all the extractions, the residues were washed with distilled water, frozen, and freeze-dried. The ammonium oxalate, sodium chloride, and 4M NaOH supernatants were recovered, dialyzed, frozen, and freeze-dried. The yields of the cell wall fractions were obtained gravimetrically. Also, to evaluate the chemical composition of the biomass samples, the infrared spectrophotometer IRPrestige-21 with the attenuated total reflectance (ATR) accessory, equipped with a germanium crystal, was used. The saccharification capacity of the cell wall from different agro-wastes were evaluated by an alkali pre-treatment (0.5 N NaOH) and enzyme blend Celic Ctec II (Novozymes®) digestion. The release sugars were measured by MBTH method (Gomez et al., 2010).

Preliminary results: The agro-wastes evaluated can be grouped as primary cell wall type I and type II regarding their polysaccharide classes levels. Nine wastes are classified as type I (soybean residue, soybean husk, soybean straw, duckweed, coffee husk, bean straw, pruning tree residues, eucalyptus chip, and industry paper residue), and ten as type II (sugarcane bagasse, sugarcane, energy cane v2, energy cane v3, rice husk, barley bagasse, corn straw, corn cob, sorghum residue, and wheat bran). Type I cell walls had, on average, 14.1% pectins, 17% pectins and soluble hemicelluloses, 23.7% hemicelluloses, 33.4% cellulose, and 11.9% lignin, while type II cell wall biomasses had 8.7% pectins, 26.3% pectin+soluble hemicelluloses, 23.5% hemicellulose, 27.3% cellulose, and 14.2% lignin. The pectin content was also indirectly determined by the uronic acid quantification, which was higher on type I cell walls (65 µg.mg-1 DW on average) than type II cell walls (44.9 µg.mg-1 DW on average).
The cell wall fractionation permitted the monosaccharides characterization of the cell wall domains. Ammonium oxalate fraction represents pectins which, type I cell walls, constituted 80% of arabinose, galactose, glucose, and xylose. Of the agro-wastes from type II walls, 90% were these sugars. In grasses (type II walls), most of the ammonium oxalate fraction comprises arabinoxylan-soluble hemicellulose and beta-glucan with high glucose levels. Sodium chloride fraction represents pectin methyl-esterified and soluble hemicelluloses. Type I cell walls of sodium chlorite fractions were xylose-rich with greater levels of arabinose, glucose, and galactose. A similar pattern was seen in to type II cell wall. In both cell wall types, more than 70% of the 4M sodium hydroxide fraction (hemicelluloses) were xylose, the other 30% differs towards biomasses. The cellulose content was evaluated by sulfuric acid hydrolysis, in which glucose was 86.6% of the residue fraction. The diverse composition reveals applications in

green chemistry, biofuels, food, cosmetics, biomedical, and pharmaceutical applications. The FT-IR allowed the molecule identification of the agro-industrial wastes by radiation´s wavelength and intensity. The 19 biomasses had a similar spectrum revealing the same characteristic peaks. However, the cellulose peak at 2290 cm-1 was more apparent in the coffee husk, which permitted the identification of the C-H bonds of caffeine 3 methyl. This methodology is useful to characterize the concentration of lignin, phenolic compounds, and cell wall composition, but is more quickly and accurate when calibrated with other methods. Sugarcane, soybean husk, corn cob, corn straw, and industry paper residue had higher saccharification capacity (23.4 mg glucose.mg CW-1) than the other tested residues. Industry paper residue, corn straw, corn cob, and soybean husk had 13 times more saccharification capacity than duckweed, sorghum residue, pruning tree residue, soybean residue, and soybean straw.

Preliminary conclusions: he chemical composition of the cell wall polysaccharides reveals diverse industrial applications of the agro-industrial-wastes, which confer a green, and sustainable option for value-added by-products in line with the circular economy. Besides that, the obtained data permits the adaptation of enzymatic cocktails for efficient pre-treatment and high yield of second-generation ethanol production.

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Abstract Title: O2 geological storage in the Paraná Basin, Brazil: an integrated assessment of unconventional reservoirs and caprocks

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Abstract: Facing the current scenario of necessary upscaling of BECCUS and CO2 geological storage to rapidly meet net-zero targets and to decarbonize the industrial and energy sectors worldwide, unconventional reservoirs gain relevance as potential CO2 reservoirs due to their widespread occurrence in Brazil and worldwide, and to their significant CO2 storage capacity. This storage capacity is associated with the microporosity and internal surface area of organic components and clay minerals in organic-rich rocks, such as shale and coal beds, which favours the adsorption trapping mechanism and promotes safe and long-term storage of CO2. In this sense, this project's contribution is to enhance the knowledge regarding potential caprocks and unconventional reservoirs for CO2 geological storage in Brazil. As a case study, this project determines the potential for CO2 geological storage of organic-rich shales of the Irati Formation

and of coal beds of the Rio Bonito Formation, Paraná Sedimentary Basin, assessing whether these are geologically feasible and safe alternatives to the onshore storage of CO2. The results are promising and show that these rocks can act both as caprocks and reservoirs of CO2 in the central, south and southeast regions of Brazil, where the BECCUS technology chain is highly applicable.

Keywords: BECCUS, CCUS, CO2 geological storage, CO2 sorption trapping, caprocks, storage system.

Introduction and Objectives: The large-scale deployment of CO2 geological storage to mitigate the worst impacts of climate change by decarbonizing the hard-to-abate sectors will require reservoir storage capacity estimates worldwide. In this sense, this research addresses the potential for storing CO2 in the Rio Bonito Formation multi lithology storage complex, composed of porous sandstones interbedded with shale and coal beds in the Paraná Basin, S and SE Brazil. Once the storage complex is defined, the safety of CO2 geological storage and containment of the reservoir relies on the caprock integrity (Busch et al., 2020; Rodrigues & Lemos de Sousa, 2002). Caprocks are usually organic-rich geological formations and their sorptive storage capacity can contribute to CO2 trapping and sequestration. Additionally, determining the storage capacity of the caprock is important to avoid misinterpretations of CO2 leakage by the potentially reducing amount of CO2 in the reservoir (Murugesu et al., 2023). In this sense, the objective of this research was to determine the CO2 storage capacity of organic-rich rocks within the Rio Bonito storage complex, and evaluate if these lithologies are feasible reservoirs and caprocks to CO2 geological storage in the Paraná Basin and favourable to CCUS technologies in the Brazilian onshore.

Methodology: To assess the CO2 sorptive storage capacity of the Irati and Rio Bonito Formations shale and coal beds, 17 representative samples were characterized in detail, through organic geochemistry (TOC, Rock-Eval pyrolysis), petrography (organofacies and vitrinite reflectance), mineralogy (XRD, SEM-EDS), porous media analysis (BET) and response to CO2 sorption isotherms (Langmuir, volumetric method).

Preliminary results: The obtained results attribute a significant storage capacity for these lithologies: 1 to 4 m3 of CO2 can be stored per tonne of shale and 5 to 7 m3 of CO2 per tonne of coal. Besides identifying the potential for storing CO2 in these rocks, in this study, the controlling factors for such storage capacity were identified and attributed to clay mineralogy, organic matter type, quantity and thermal maturation.

Preliminary conclusions: Based on integrated data interpretation, we concluded that these organic and clay-rich lithologies configure both caprocks and unconventional reservoirs to CO2 storage due to this significant capacity of trapping CO2 through adsorption into clay minerals and organic particles. Additionally, we identified thermal maturity as the main controlling factor of shale and coal sorptive storage capacity. This is demonstrated in samples that went

through contact metamorphism due to their proximity to igneous intrusions, which are attributed to the Serra Geral magmatism and characteristic of the Paraná Basin. Finally, we established a research methodology for determining the CO2 storage capacity of organic-rich lithologies, which can be replicated in other sedimentary basins worldwide.

Jessica Santos Rego
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Abstract Title: CO2 adsorption on representative feldspar mineral surfaces by first-principles calculations

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Abstract: Concerns over climate change resulting from greenhouse gas emissions, such as carbon dioxide (CO2), have prompted the search for technologies capable of mitigating their impact. One promising alternative is geological capture and storage through carbonation reactions. The Rio Bonito formation in the Paraná basin in Brazil appears to be a suitable location for implementing this technology. Molecular-scale simulations are crucial for understanding the mechanisms and processes involved in fluid/mineral interfaces at the geological site reservoir. Using Density-Functional-Theory (DFT), we evaluated the adsorption behaviour of CO2 molecules on selected mineral surfaces, namely feldspar. We focused on preferential feldspar's cleavage plane surfaces, {010} and {001}. We quantified and compared the electronic and thermodynamic properties of different adsorption configurations from an energetic and topological perspective. We also explored the determination of preferential adsorption sites and the influence of the aqueous environment on adsorption. Our simulations provide valuable insights into the intricate interactions occurring at complex CO2 mineral interfaces under reservoir conditions. This work was carried out with support from Shell and FAPESP (grant 2022/08894-0, RCGI 2020/15230- 5, São Paulo Research Foundation (FAPESP).

Keywords: CO2, mineralisation, carbon storage, CCS, BECCUS.

Introduction and Objectives: he growing concern about climate change caused by the emission of greenhouse gases (GHG) into the atmosphere, including carbon dioxide (CO2), has spurred the quest for technologies capable of mitigating the impact of these pollutants. Among the promising alternatives, carbon capture and storage through geochemical trapping, achieved

via mineralisation, has emerged as a viable solution. Due to its unique composition and physicochemical properties, the Rio Bonito Formation (located in South America, Paraná Basin) has enormous potential for CO2 storage through mineral carbonation. In contrast to similar sandstone formations in North America, the Rio Bonito Formation contains a relatively higher amount of K-feldspar, plagioclase feldspar, and smectite, in combination with excellent permeable properties and suitable pressure-temperature confinement conditions for CO2 storage. However, further studies are still needed to model and select the ideal reservoir conditions for this specific site and conduct additional investigations into CO2 mineralisation reactions at the molecular and pore scales. Ensuring the viability and environmental sustainability of using the Paraná Basin as a reservoir for geochemical trapping of CO2 requires overcoming challenges and understanding the practical limitations of applying existing technology. This involves the initial crucial step of comprehending the geochemical reactions essential for evaluating CO2 trapping mechanisms in selected reservoirs and their impacts on performance. Robust interdisciplinary collaborations and a multi-level approach are imperative to mitigate environmental impacts and enhance the efficiency of geological carbon storage (GCS) operations. Firstly, it is important to emphasise that the geological storage of carbon in sandstones constitutes a multicomponent system, comprising injected CO2, brine, and the minerals constituting the pore system. The interfaces between all these components and their interactions under spatial confinement are dominated by surface effects. The sorption process plays a crucial role in the carbonation reaction and CO2 trapping mechanisms, particularly in the geological storage of CO2. The sorption of CO2 onto mineral surfaces can significantly enhance the carbonation reaction by increasing the concentration of dissolved CO2 in the aqueous phase. Additionally, trapping by adsorption is particularly important for low-permeability rock formations where CO2 cannot migrate through the rock matrix. Hence, this study aims to delve into the nano-scale molecular level to explore the CO2 sorption potential of select representative minerals within the context of mineral trapping and CO2 plume migration.

Methodology: The initial step entailed selecting representative minerals for our simulations. After consulting with geologists conducting petrographic characterisation of Rio Bonito Formation samples, mineralogical analysis revealed that the most abundant feldspars in the Rio Bonito Formation are microcline and albite, with some oligoclase also present. However, we also decided to include anorthoclase due to observed heterogeneity in these formations. These selected minerals' initial crystal structure configurations were obtained from experimental databases such as the Inorganic Crystal Structure Database (ICSD) and the American Mineralogist Crystal Structure Database (AMCSD). All calculations were performed using Density Functional Theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP). We utilised the optB88-vdW exchange-correlation functional with dispersion correction and employed the corresponding projector augmented wave (PAW) scheme, treating specific electron configurations as valence states. A kinetic energy cutoff of 800 eV was applied for the plane-wave expansion of the Kohn-Sham orbitals, and we sampled the Brillouin zone using the Monkhorst-Pack scheme. As a first step, all structures underwent relaxation using

conjugate-gradient energy minimisation, allowing for optimisation of both the ionic degrees of freedom and the cell volume and shape. The energy tolerance for the self-consistency cycles was set at 10e−6 eV. The convergence criteria for energy minimisation were established to ensure that the maximum residual magnitude of atomic forces and stress components remained below 0.001 eV/Å. After unit cell optimisation, 2x1x2 supercells were constructed, and the same protocol was applied.
To calculate adsorption energies, it was necessary to identify the low-index surfaces of each crystal, i.e., the cleavage planes of the minerals. Based on the literature, we selected the {010} and {001} surfaces for the feldspar minerals to investigate in the subsequent steps. After obtaining optimised unit cells, three-dimensional periodic slab models were employed to simulate infinite surfaces. 2x1x2 supercells of the minerals were created for this purpose. In constructing the surface structure, the atoms at the bottom of the first two layers were fixed. A vacuum thickness of 15 Å was set to ensure minimal surface-surface interaction. The Brillouin zone was sampled at the Gamma point, and the energy cutoff was set at 600 eV. The adsorption energy of CO2 molecules at different sites on the {001} and {010} faces of the feldspar layers was evaluated using the complex-minus-fragment method.

Preliminary results: he structures of CO2 molecules adsorbed on the selected mineral surfaces were obtained through geometry optimisation calculations. For each surface, we considered seven different adsorption sites. In all calculation scenarios, CO2 molecules were adsorbed on the surfaces in their molecular form. Notably, we observed negative energy values for all configurations across all sites, indicating favourability for CO2 adsorption. The most favourable site, characterised by the most negative adsorption energy, corresponds to the configuration where the CO2 molecule interacts most directly with the aluminium atom on the feldspar surface. Another crucial analysis involves classifying the adsorption phenomenon's behaviour as physical adsorption (physisorption) or chemical adsorption (chemisorption). The primary distinction between these processes lies in the nature and strength of the forces involved, both critical in geological carbon storage. Chemisorption entails the formation of strong chemical bonds and is characterised by a high activation energy requirement. In contrast, physisorption is governed by weaker intermolecular forces and has a lower activation energy requirement. Chemisorption typically results in forming a monolayer of adsorbate molecules, while physisorption can lead to the formation of multilayers. Chemisorption is generally considered irreversible, while physisorption can be reversed under suitable conditions. Physical adsorption is more closely related to the reservoir's storage capacity, while chemical adsorption is associated with long-term storage through carbonation. Therefore, it is imperative to comprehend the distinct sorption mechanisms and their interactions with minerals to optimise and enhance carbon capture and storage technologies. We analysed structural and electronic parameters to determine the type of sorption process occurring on the surface of feldspar for CO2 molecules. Consistent with the existing literature, structural parameters such as variations in bond lengths and angles of CO2 between its gaseous state and the adsorbed state serve as critical indicators of the underlying process. Minor structural distortions typically imply physical adsorption, whereas substantial distortions signify chemisorption. Our findings reveal

that the geometric distortions of the CO2 molecule are minimal, implying a physical adsorption process. Other parameters used for sorption characterisation include charge differences between the adsorbate and the surface and interaction energy values between the atoms with the strongest interactions on the surface. Our analysis yielded charge density difference values ranging from approximately 0.03 to 0.01e, considered small and indicative of physical adsorption. Furthermore, when examining the interaction energy values of the atoms, we found values in the range of 0.10 to 0.05 eV, once again reinforcing the conclusion of physical adsorption.

Preliminary conclusions: This investigation delves into the adsorption characteristics of CO2 on select representative feldspar minerals using density functional theory. We have observed that all these minerals possess multiple surface sites capable of adsorbing CO2 molecules. We find strong indications of physisorption behaviour by analysing additional properties such as geometric distortion, the partial density of states, and atomic charge redistribution of the mineral surfaces before and after CO2 adsorption. Physisorption suggests that CO2 exhibits a weak interaction with the mineral surface, enabling molecules to be easily absorbed or released from the mineral surface by modifying temperature, pressure, or other external factors. This reversibility is a distinctive feature of physisorption, setting it apart from chemisorption, where strong chemical bonds form, and adsorption is generally irreversible under mild conditions. In applications like geological carbon capture and storage, several layers of carbon dioxide can be adsorbed onto mineral surfaces in porous geological formations, contributing to the CO2 storage capacity in the subsurface. Physisorption processes also find utility, for instance, in gas storage within porous materials such as activated carbon or zeolites, enabling the adsorption and storage of gases like methane or hydrogen. However, it is worth highlighting that minerals demonstrating chemisorption are also noteworthy due to their relevance in processes like mineral carbonation. In mineralisation, CO2 undergoes a chemical reaction with specific minerals, forming stable carbonate compounds, effectively storing CO2 in a more enduring and geologically stable form—carbonate minerals. The findings of this study provide a fundamental understanding of the adsorption mechanism for CO2 in these minerals. The information presented here may serve as a computational framework, including procedures and analyses, to assess the CO2 sequestration potential of other representative minerals.

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Abstract Title: Water confined by silica Slits

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Abstract: Understanding water properties at the nanoscale, particularly within confined spaces

such as displayed by silica nanochannels, is an emerging research area with implications spanning numerous scientific domains. It is well established that the unique environment within silica nanochannels can significantly alter the water properties, thus presenting an opportunity to leverage this to manipulate water characteristics for desired outcomes. In this study, we delve into the molecular dynamics of water spatially confined in silica nanochannels, exploring how the water-silica interface impacts the water structure and dynamics. By performing extensive simulations grounded in the classical molecular dynamics, we describe the water features under confinement including hydrogen bonding patterns, density profiles, and diffusion coefficients.

Keywords: silica nanochannels, molecular dynamics simulations, hydrogen bonding.

Introduction and Objectives: Over the past decade, the fast-paced development in nanotechnology has escalated the interest in understanding the confined water features. Fluids may display distinct properties at the nano-interface, a domain where the traditional macroscale theories falter, presenting fertile ground for groundbreaking research. The urgency to understand this confinement effect also stems from its broad applicability in biosensing, nanofluidics, and environmental science, where water manipulation at the nano-scale could potentially revolutionize existing technologies. The focus of this study is thus on explore confinement effects on water concerns parameters like density profiles, self-diffusion, T2 relaxation time, and hydrogen bonds, utilizing the ever-evolving tools of molecular dynamics, which is primed to offer fresh insights into the mechanisms at play in silica-water confinement scenarios. A critical aspect of this endeavor will be to unravel the underlying principles guiding the behaviour of hydrogen bonds in this constrained environment, a key player in the physical properties of confined water. Furthermore, elucidating the role of T2 relaxation time in this setting offers a pathway to grasp the transient behaviours and associated dynamics.

Methodology: We employed the Grand Canonical Monte Carlo (GCMC) method utilizing the Cassandra software to facilitate the equilibration process of filling the silica plates pore model with water molecules. This preparatory step ensured the establishment of an optimal molecular configuration to accurately replicate the complex environment of water confined between silica plates. Following this, a two nanoseconds (ns) simulation in the canonical ensemble (NVT) was conducted using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). These allowed to further equilibrate the system and achieve a stable state. This progression led to the paramount phase of the study, where a meticulous ten ns simulation for the production state was undertaken in the NVT ensemble to glean the properties of confined water at the silica interface. The simulations were structured to capture pivotal parameters such as density profiles, self-diffusion, T2 relaxation times, hydrogen bonds, and interfacial tension, yielding insights that stand to be the bedrock of our comprehensive analysis.

Preliminary results: In the ensuing analysis of the simulation data, a pronounced influence of confinement water features on several pivotal parameters was unveiled. Firstly, a notable

impact on the T2 relaxation time was observed, illustrating the pronounced effect of the confined environment on the water molecules' dynamical properties. The interfacial tension (IFT) exhibited substantial variations, highlighting the crucial role played by the interface in dictating the water properties as observed also on the density profile. Furthermore, the self-diffusion properties underwent notable changes, illustrating the marked effect of silica-water interactions on the mobility of water molecules within the confined space. These findings collectively spotlight the significant bearing of confinement on the intrinsic properties of water, setting a promising stage for forthcoming studies to delve deeper and fully unravel the complexities of water behaviour in silica nanochannels. This establishes a rich groundwork for further research, aiming to build a comprehensive understanding that can fuel innovations in nano-confined fluid dynamics and offer a nuanced view that could redefine our understanding of fluid behaviour at the nanoscale.

Preliminary conclusions: n conclusion, this study has delineated the influence of spatial confinement on pivotal aspects such as T2 relaxation times, interfacial tension, density profiles, and self-diffusion in water-silica nanochannel systems. The findings accentuate the intricate dynamics at the nano-interfaces, revealing a realm of complex interactions and phenomena distinct from bulk behaviours. As we stand on the threshold of deeper understanding, the path forward beckons, integrating even more complex systems into our study domain. Future endeavours should strategically pivot towards incorporating ionic species in confinement simulations to unravel the impacts of electrostatic interactions and ion-specific phenomena in confined environments. Furthermore, the exploration should extend to examining cylindrical structures, venturing beyond planar geometries to delineate the confinement effects in different topological settings. This progression promises a richer understanding of the confinement phenomena and opens the potential to unearth novel applications and technologies.

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Abstract Title: The feasibility of carbon capture technologies in wastewater treatment plants in Brazil

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Abstract: In a scenario in which climate change, caused mainly by human actions, has become a global problem, both in terms of the environment and in terms of human health, new methods

and technologies are sought to minimize these impacts and solve these environmental problems. The purpose of the study is to investigate the pros and cons of implementing technologies for carbon capture in wastewater treatment processes in Brazil. Furthermore, it indicates the scenarios that favour the use of bio electrochemical systems. Considering that these innovations are recent, the cost is the biggest challenge for implementation, especially in a developing country, such as Brazil.

Keywords: Bio electrochemical systems, carbon capture, wastewater treatment.

Introduction and Objectives: Bio-electrochemical systems, also known as BESs, are technologies that, through the use of microorganisms as catalysts, convert chemical energy into electrical energy. Through these processes, it is possible to capture carbon dioxide (CO2) and generate desirable products, such as H2 gas that can be used for energy purposes. Among the types of technologies that are based on BESs are microbial carbon fuel cells (MCCs), microbial fuel cells (MFCs), plant-based microbial fuel cells (P-MFCs), microbial electrolysis cells (MEC) and microbial electro-synthesis cells (MESs). The main objective is to contribute to the understanding of the opportunities and difficulties, in the case of Brazil, in implementing carbon capture in wastewater treatment plants.

Methodology: The methodology was a systematic literature review. Firstly, it was made an advanced search using the keywords “bio electrochemical systems, carbon capture, wastewater treatment”. Subsequently, the official Brazilian Qualis/CAPES system was used, with the aim of classifying scientific production and the most qualified articles were kept. Finally, the scientific journals were read and studied to understand the favourable and unfavourable scenarios of BESs technologies.

Preliminary results: Considering that these technologies are recent, the cost, biggest challenge for implementation, can be reduced if there are changes such as design optimizations.

Preliminary conclusions: Bio electrochemical systems (BESs) are recent innovations that have high potential to participate in environmental solutions. One of the biggest challenges for Brazil is the financial cost.

Vitor Favaretto Pinoti
State Univerisity of Campinas/University of Sao Paulo

Abstract Title: Development of CRISPR-based gene editing tools and identification of herbicide resistance endowing target mutations in sugarcane

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Abstract: Climate changes are demanding worldwide nations to lower their greenhouse gas

emissions by shifting their energy matrixes to biofuel-based ones. Sugarcane is considered the ideal crop for biofuel production, but weed management still poses major loses to sugarcane production. Biotechnology may leverage classical breeding approaches, and CRISPR technologies expanded precise genome editing possibilities. Therefore, establishing an efficient CRISPR-mediated genome editing pipeline to create new herbicide resistant varieties would increase sugarcane production. In the present, we present a series of vectors for executing CRISPR-mediated genome editing in sugarcane. Specifically, we provide vectors for classical indel knockouts and for specific alterations by base editing, prime editing and HDR approaches. Additionally, a vector set for straightforward gRNA units cloning by Golden Gate assembly was also constructed. Moreover, we also identified novel herbicide resistance endowing mutation within the ALS and EPSPS genes from sugarcane. Collectively, our work presents cutting-edge breeding techniques along with new options for weed management in sugarcane.

Keywords: Gene editing; CRISPR; sugarcane.

Introduction and Objectives: Climate changes are demanding a worldwide effort to lower greenhouse gas emissions by shifting the energy matrixes to biofuel-based ones. Sugarcane is considered the ideal crop for biofuel production. In spite of transgenesis-based technologies being widely used in agriculture, CRISPR-based technologies have opened a wide array of new possibilities of precise genome editing. Specifically, cutting-edge techniques such as base editing and Prime editing allow the installation of point mutation that can provide either gain or loss of gene functions. Sugarcane, a complex polyploid, poses several a challenge for gene editing, due to a high number of alleles. Moreover, since sugarcane is vegetatively propagated, the segregation of transgenes used to introduce gene edits, is not a viable option. Gene edited plants, without the incorporation of transgenes, have simple regulatory approval process. Therefore, a transgene-free genome editing protocol would boost sugarcane improvement. Gene edits that make plant cells resistant to herbicides can be used as a strategy towards this goal. It is worth mentioning that herbicide resistant plants per se would be useful for farmers, since this would easy the weed control with herbicides are a major problem. Accordingly, the present work aims to establish efficient CRISPR-mediated genome editing tools and prospect herbicide resistance endowing target mutations in sugarcane.

Methodology: ScPDS, ScALS, SCEPSPS and ScGS1 sequences: The genomic sequences and coding sequences (CDSs) phytoene desaturase (PDS), Acetolactate synthase (ALS), -enolpyruvylshikimate-3-phosphate synthase (EPSPS) and Gluthamine systhetase1 (GS1) genes from sugarcane cultivar SP80-3280 were obtained from publicly available databases from SUCEST and NCBI. The ScPDS, ScALS, ScEPSPS and ScGS1 coding sequences were PCR amplified, cloned into pGEM-T-easy vector and sequenced by Sanger method. roduction of transgenic plants overexpressing herbicide target genes coding sequence with resistance endowing mutations: The coding sequences of ScALS, ScEPSPS and ScGS1 genes bearing herbicide resistance endowing mutations were constructed by overlap PCR. After sequencing, the mutant versions were cloned into the pGVG vector and transformed in SP80-3280

sugarcane variety by Pangeia Biotech. After acclimatation, transgenic events overexpressing ScALS and ScEPSPS mutant versions were challenged with commercial doses of Imazapyr and Glyphosate herbicides, respectively, and phytotoxicity was visually scored. Production of transgenic plants carrying CRISPR reagents: The CDSs of SpCas9 (Cas9), nSpCas9(D10A)-PmCDA1 (TargetAID) and nSpCas9(H840A)-NC-M-MLV Delta RNase H (ePPE) were cloned into the pGVG vector by restriction ligation reactions. Subsequently, the gateway cloning cassette encompassing the CmR-ccdB region flanked by Att1 and AttR2 sites was cloned into the pGVG vectors by restriction ligation reactions. RAD51DBD-ABE8e-nSpCas9(D10A) (ABE). After receiving the sgRNA expression units, the pGVG-Cas9 and pGVG-TargetAID vectors were transformed into SP80-3280 sugarcane variety by Pangeia Biotech thought their proprietary agrobacterium-mediated genetic transformation method. SgRNA design and cloning: sgRNA design for base editing and gene targeting were done with the Benchling and CRISPOR online tools, respectively. Oligos carrying the selected target sequences were ordered and used to generate PCR fragments bearing sgRNA elements. Afterwards, the PCR fragments were cloned into intermediate gateway cloning vectors thought Golden Gate assembly and then transferred into pGVG vectors by LR reactions. Identification of edited events: To identify edited events among pGVG-TargetAID-ScALS transgenic plants, PCR followed by Restriction Enzyme (PCR-RE) method was used. Genomic DNA from transgenic plants was extracted and the A96V target region within the ScALS was PCR amplified with flanking primers. PCR products were then digested with the HhaI restriction enzyme, which is sensitive to the cytidine change installed by the TargetAID nuclease that generates the herbicide resistance endowing mutation in the ScALS gene. Restriction digestion products were resolved in agarose gels and samples with undigested fragments were cloned in pGEM-T-easy vectors and sequenced by Sanger method. Sequencing results were manually analysed in the SnapGene tool.

Preliminary results: In the present work, we sought to identify herbicide resistance endowing mutations in the ScALS and ScEPSPS genes that could be installed by CRISPR methodology. After challenged with Imazapyr and Glyphosate herbicides, highly resistant plants overexpressing ScALS or ScEPSPS mutant versions were obtained, respectively. In parallel, we constructed a vector set for CRISPR-mediated genome editing in sugarcane. Thus, CDSs of the CRISPR nucleases Cas9 and TargetAID were cloned into the pGVG vector, thus generating the vectors to be used for classic indel knockout and cytidine base editing (CBE), respectively. Furthermore, the gateway cloning cassette was added to the aforementioned constructs to permit sgRNA expression units cloning through LR reaction. Moreover, minor modifications in the Plant Molecular Cloning (MoClo) system based on the Golden Gate assembly method yielded an assembling strategy for multiplexing sgRNA cloning under the control of polymerase II promoter. Furthermore, we deployed the PmeI restriction site in pGVG-Cas9 vector for homology-directed repair template cloning and HDR experiments. To test our vector set, we selected the phytoene desaturase (PDS) gene since its knockout renders an albino phenotype. After CRISPR vectors assembly and sugarcane transformation, we observed only one transgenic event presenting an albino phenotype thus indicating low levels of multiallelic editing required for ScPDS knockout. Currently, molecular analyses to evaluate TargetAID and

Cas9 systems performance within ScPDS gene are being conducted. Additionally, a TargetAID construct to install the previously identified herbicide resistance endowing mutation in the ScALS gene was also transformed into sugarcane. However, we did not obtain resistant transgenic events after challenging with Imazapyr herbicide. Interestingly, PCR-RE analyses revealed the occurrence of indels instead of correct editing in the ScALS gene target region, which is a common by-product of the CBE system. Altogether, these results indicate that CBE system presents low levels of correct editing in sugarcane. To conceive high efficiency editing systems and additional herbicide endowing target mutations, we constructed additional vectors for executing Prime editing (PE) and adenosine base editing (ABE) systems, which present elevated editing efficiency in monocotyledonous plants. To test the PE and ABE systems, we selected another mutation in the ScALS gene and a mutation in the ScGS1 gene, which confer Imazapyr and Glufosinate resistance, respectively. Currently, transgenic plants individually overexpressing ScGS1 and the new ScALS mutant versions are being produced and will be challenged with Glufosinate and Imazapyr after acclimatation, respectively. Lastly, transgenic plants carrying a construct to install the previously identified herbicide resistance endowing mutation in the ScEPSPS gene thought gene targeting (HDR) were generated and will be challenged with Glyphosate soon.

Preliminary conclusions: In the present work, a variety of DNA vectors for CRISPR-mediated genome editing were built allowing the execution of classical indels as well as point mutation by base editing. Additionally, the Prime editing and gene target vectors provided here allow complex mutations, such as multiple interspaced base changes and large insertion/deletion. Along with our sgRNAs cloning strategy, this vector set represents a complete CRISPR-mediated genome editing vectors toolbox for sugarcane research and improvement. Our preliminary cytidine base editing tests indicate that the nSpCas9(D10A)- PmCDA1 (TargetAID) system had low efficiency in sugarcane in comparison to what was observed in other monocotyledonous plants. Therefore, we are testing other cytidine base editing systems to provide elevated efficiency for this type of gene editing modality in sugarcane.
In addition to the CRISPR-mediated genome editing vectors toolbox presented here, we also identified Imazapyr and Glyphosate endowing target mutations within the ScALS and ScEPSPS genes, respectively. Moreover, we are also testing new target mutations to be installed by Prime editing and adenosine base editing within ScALS and ScGS1 genes, respectively. Therefore, in addition to cutting edge breeding techniques, the present work also provides novel sugarcane specific mutant version of herbicide target genes for weed management.

Verena Mandorino Kaminagakura
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Abstract Title: Energy generation in microbial fuel cell in the treatment of vinasse, removal of organic matter and nitrogen

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Abstract: One of the biggest current challenges is the development of technologies that seek to meet energy demand and wastewater treatment. In this context, microbial fuel cells (MFC) present themselves as a promising technology, as they allow the conversion of chemical energy, originating from various substrates, such as vinasse, to electrical energy. However, this process has some limitations and challenges that needs to be addressed in order to increase energy production and improve treatment efficiency. This investigation aimed to evaluate the use accessible and low-cost electrodes, based on granular activated carbon, in power generation, removal of organic matter, nitrification and autotrophic denitrification in the treatment of vinasse. The dual-chamber and continuous feed MFC were divided into 3 types: MFC control, MFC nitrifying and MFC denitrifying. The efficiency of the system was evaluated by physicochemical and electrochemical parameters and the biofilm obtained was subjected to molecular biology analyses. The average COD and TOC removals obtained were: 81% COD and 80% for MFC control, 78% COD AND 79% TOC for MFC nitrifying and finally, the highest average removal of 85% COD and 87% of TOC was achieved with MFC denitrifying, using nitrate as an electron acceptor. The average total nitrogen removal for MFC control was 19%, for MFC nitrifying it was 39.3%, and for MFC denitrifying the average total nitrogen removal was 5.8%. In terms of energy generation, the maximum power densities were 3.65 W.m-3, 1.06 W.m-3 and 0.59 W.m-3 for MFC control, MFC nitrifying and MFC denitrifying, respectively. The Coulomb efficiencies were 2.46% for MFC control, 0.28% for MFC nitrifying and 1.35% for MFC denitrifying.

Keywords: bioenergy, nitrification, denitrification, MFC, vinasse.

Introduction and Objectives: One of the biggest current challenges is the development of technologies that seek to meet energy demand and wastewater treatment. In this context, microbial fuel cells (MFC) present themselves as a promising technology, as they allow the conversion of chemical energy, originating from various substrates, such as vinasse, to

electrical energy. However, this process has some limitations and challenges that needs to be addressed in order to increase energy production and improve treatment efficiency. This investigation aimed to evaluate the use accessible and low-cost electrodes, based on granular activated carbon, in power generation, removal of organic matter, nitrification and autotrophic denitrification in the treatment of vinasse.

Methodology: An MFC was developed based on a compact dual-chamber design with low-cost electrodes. The experimental study is composed of 3 phases, phase 1: Development of the MFC; Phase 2: Inoculation and stabilization; Phase 3: System evaluation.

2.1 Development of MFC – Phase 1

The dual-chamber MFC was designed with the aim of obtaining a compact model, with chambers of the same volume. To accurately meet the needs, the Autodesk Inventor Professional 2012 software was used. The project was executed on a 3D printer model Flashforge dreamer NX, using acrylonitrile butadiene styrene (ABS) filaments.

2.2 Inoculation and stabilization – Phase 2

1 MFC control, 1 MFC nitrification and 1 MFC denitrification were started independently. Seeking a system with high microbiological diversity, the anode chambers were inoculated with 50% of the GAC coming from another MFC fed with synthetic vinasse wastewater that operated in continuous feeding mode for 18 months and 50% of virgin GAC. The control MFC, with aerated cathode and fed with phosphate buffer solution (PBS) without inoculation. To evaluate the bioelectrochemical nitrification and denitrification process associated with the cathode, they were inoculated as the anode. The cathodes of the MFC control and MFC nitrification continue aeration. The catholyte was composed of synthetic vinasse without the organic fraction, supplemented with ammonia for MFC nitrification, and nitrate for MFC denitrification. The operation was carried out at room temperature, with 300 Ω external resistance (Rext) and hydraulic retention time (TDH) of 33 hours for each chamber and continuous feeding (CANO et al., 2023).

2.3 System evaluation – Phase 3

The treatment efficiency for removing organic matter and nitrogen was evaluated using the parameters in the Standard Methods for the Examination of Water and Wastewater (APHA, 2022). Among them, the main parameters are: COD, Total organic carbon (TOC), Total nitrogen, selective ion chromatography, pH and conductivity. Energy generation was evaluated using electrochemical data obtained with polarization curves, electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV).

Preliminary results: The average COD and TOC removals obtained were: 81% COD and 80% for MFC control, 78% COD AND 79% TOC for MFC nitrifying and finally, the highest average removal of 85% COD and 87% of TOC was achieved with MFC denitrifying, using nitrate as an electron acceptor. The average total nitrogen removal for MFC control was 19%, for MFC

nitrifying it was 39.3%, and for MFC denitrifying the average total nitrogen removal was 5.8%. In terms of energy generation, the maximum power densities were 3.65 W.m-3, 1.06 W.m-3 and 0.59 W.m-3 for MFC control, MFC nitrifying and MFC denitrifying, respectively. The Coulomb efficiencies were 2.46% for MFC control, 0.28% for MFC nitrifying and 1.35% for MFC denitrifying.

Preliminary conclusions: All MFC prototypes showed efficiency above 80% in organic matter removal and nitrogen removal performance during the monitoring period. This indicates that they all developed a biofilm capable of removing organic matter, regardless of the catholyte. Total nitrogen removal was 19% and 39% for nitrifying MFC and denitrifying MFC. As for energy generation, adjustments to the proposed project were necessary to improve efficiency, where the low values were, quite possibly, associated with poor electrical contact of the electrodes.

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Abstract Title: High power density Solid Oxide Fuel Cells on the temperature range of 400-700 ºC, an overview.

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Abstract : This work presents an overview of the state of the art of solid oxide fuel cells (SOFC) with respect to power density when operating at a temperature range of 400 – 700 ºC. Inside the SOFC, three different subcategories have been classified as Solid Oxide Fuel Cell typical, (SOFCt), Protonic Ceramic Fuel Cell (PCFC), and Semiconductor-ionic Membrane Fuel Cell (SIMFC) and compared in terms of maximum power density (MPD). The highest MPD values for each fuel cell technology found in the temperature range investigated were 3270[1], 1900[2] and 1296[3] for SOFC, PCFC and SIMFC, respectively.

Keywords: SOFC; PCFC; SIMFC; power density.

Introduction and Objectives: Solid oxide fuel cells are ceramic devices that can efficiently generate electricity from electrochemical reactions, are relatively tolerant to fuel contamination and flexible with respect to fuels that can be used. It was discovered by Nernst, in 1899, and

several subcategories, such as Protonic Ceramic Fuel Cell (PCFC), Semiconductor-ionic Membrane Fuel Cell (SIMFC), and Electrolyte Free Fuel Cell (EFFC), among others, have been developed since then[4]. The objective of this work is to compare the performance of three subcategories of SOFC, named SOFCt, PCFC and SIMFC in terms of power density, from 128 papers published. Hence, the highest peak power density (or maximum power density, MPD, published for the cases where the peak power was not achieved) of each work has been considered into the analysis. In addition to that, this work is focusing on the transportation segment, with the use of ethanol, which makes us believe the operating temperature range of 400 – 700 ºC could be ideal[5]. The effects of operating temperature and electrolyte thickness on the MPD are also being analysed.

Methodology: Since not all papers differentiate the SOFC into subcategories, in this work, the following differentiation criterion was used to compare the results between these three ceramic fuel cell types. Most but not all the criteria must be met in order to conclude the classification.

- SOFCt

Electrolyte is conductive only to O2-;

Ideally, the electrical conductivity of the electrolyte is zero or neglected;

Highly dense electrolyte;

High sintering temperatures;

Absence of metals in the electrolyte;

MPD has a positive correlation with operating temperature.

- PCFC

Electrolyte is conductive only to H+;

Ideally, the electrical conductivity of the electrolyte is zero or neglected;

Highly dense electrolyte;

High sintering temperatures;

Absence of metals in the electrolyte;

MPD has a positive correlation with operating temperature.

Differently from the SOFCt and PCFC, the SIMFC doesn't need to have a 3-layers architecture, and it could work without electrolyte. In order to properly work, an electrical barrier needs to take place, hindering short-circuits, since the electrode materials of the SIMFC need to be conductive to both electrons and ions.

- SIMFC

N-p heterojunction or similar;

- Schottky barrier;

- NCAL-Ni as both cathode and anode;

Lower sintering temperature;

Nanoparticles in electrolyte;

Electrolyte is not as dense;

Thick electrolyte;

Highest MPD at or near 550 oC;

Electrolyte has both ionic and electronic conductivity;

Conductive to H+ and O2-.

Preliminary results: Fig. 1 shows the MPDs reported on 128 papers for three types of fuel cells: SOFCt, PCFC and SIMFC. The highest MPD values for each fuel cell technology found in the temperature range searched were 3270[1], 1900[2] and 1296[3] for SOFC, PCFC and SIMFC, respectively.

Fig. 1 - Maximum Power Density of 128 studies reported with H2 vs operating temperature.

The lines in Figure 1 represent the weighted histograms, which were calculated by the normalized sum of MPD for each fuel cell type at each temperature. As the MPD of SOFCt and PCFC show a positive correlation with temperature, the MPD of SIMFC has a peak in 550 ºC, indicating it is a different technology. Moreover, over 80% of all the MPDs found in the literature are at this temperature. This behavior can be explained by the efficiency loss of the Schottky barrier effect, which prevent from electrons flowing in the wrong direction, with the temperature increase[6-8]. Although the SIMFC did not achieve the highest MPD values at 550 ºC, MPDs higher than 1 W cm-2 were reached, which is comparable to the highest PCFC and the second highest SOFCt MPD values for this temperature. It can also be observed in Fig. 1 that the SOFCt has higher MPD values at all operating temperature, which is an indicative that this technology is more mature. Ju et al. studied MS-SOFCs with a dense nanofilm as an advanced anode and achieved a MPD of 2.95 W cm-2 at 700 ºC[9]. By using a cost effective manufacturing process, screen-printing, Joh et al. obtained a MPD of 2.08 W cm-2 with a ~12 um bilayer ESB/YSZ electrolyte on an anode supported SOFC, operating at 700 ºC. PCFCs are gathering increasing interest due to the lower activation energy for proton conduction which enables lower operating temperature, but at lower temperatures, cathodic polarization losses become more prominent. Seong et al. studied the effect of cathode microstructure and noted that with the intermediate cathode porosity studied of 53%, the cathodic resistance reduced ~38%, resulting in a PPD 32% higher[11].

The effect of electrolyte thickness on the MPD was also analyzed and the 10 highest MPD results of each fuel cell type versus the electrolyte thickness are shown in Fig. 2.

Fig. 2 – 10 highest MPD vs Electrolyte thickness for SOFCt, PCFC and SIMFC, on H2.

Figure 2 shows a clear segregation between SIMFC from the others in terms of electrolyte thickness. That indicates that the electrical performance of both SOFC and PCFC is inversely correlated to the ohmic loss and area specific resistance (ASR), which doesn't seem to be the case for the SIMFC. Although, this analysis has a limitation and once a thin film electrolyte can be

successfully fabricated, the performance of electrodes, especially the cathode, becomes more important than further reducing the electrolyte thickness[12-13]. The biggest challenge for the SIMFC to be used in the transportation area is to significantly reduce its overall thickness, that implies lower gravimetric power density.

Preliminary conclusions: It can be inferred from this study that the SOFCt is the technology with higher maturity level, therefore achieved higher MPD results. The biggest challenge for the SIMFC technology in this application is to reduce its overall thickness.

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0811 - CCUSS7 (TV3)

Chairs: Lucy Gomes Sant Anna – Renato Gonçalves

Dielle Pierotti Procópio
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Abstract Title: Conversion of CO2 into biopolymers by the regulation of polyhydroxyalkanoate (PHA) biosynthetic pathway using the photosynthetic cyanobacteria Synechocystis sp.

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Abstract: Isolated from the mangrove region of Brazil, the efficient strain of the cyanobacterium Synechocystis sp. B12 showcases a remarkable capacity to produce poly(3-hydroxybutyrate) (PHB) at a substantial level of 31% cellular dry weight, even under the intense light conditions of 300 µmol photons m-2 s-1. Such attributes hold promise for applications in the field of biotechnology. Through the analysis of the 16S rRNA gene sequence, the B12 strain was conclusively categorized within the Synechocystis genus. To enhance our understanding of Synechocystis sp. B12's DNA sequence, its genome was obtained by employing a minION nanopore-based sequencing platform known for its longer-read capabilities, alongside the metaFlye algorithm assembly. This approach aimed to uncover the organism's metabolic pathways and identify the genes accountable for polyhydroxyalkanoate (PHA) production. The exhaustive genome sequencing of strain B12 revealed a circular chromosome spanning 4.05 Mbp. Among the discerned genetic elements were those associated with PHA metabolism, carbon utilization, and energy production. These genetic signatures were then juxtaposed against analogous species' metabolic profiles, providing valuable insights. Detailed annotation of the identified genes demonstrated the presence of typical PHA biosynthesis-related genes such as phaA, phaB, phaE, and phaC. This comprehensive evaluation facilitated an initial comprehension of their organizational framework. Furthermore, a comprehensive exploration identified regions potentially encoding proteins through a similarity search, ultimately yielding a comprehensive prediction of 5,290 genes.

Keywords: bacterial energy storage, biodegradable plastic, biopolymers, carbon capture, polyester.

Introduction and Objectives: Isolated from the mangrove region of Brazil, the efficient strain of the cyanobacterium Synechocystis sp. B12 showcases a remarkable capacity to produce poly(3-hydroxybutyrate) (PHB) at a substantial level of 31% cellular dry weight, even under the intense light conditions of 300 µmol photons m-2 s-1. Such attributes hold promise for

applications in the field of biotechnology. Through the analysis of the 16S rRNA gene sequence, the B12 strain was conclusively categorized within the Synechocystis genus.

Methodology: To enhance our understanding of Synechocystis sp. B12's DNA sequence, its genome was obtained by employing a minION nanopore-based sequencing platform known for its longer-read capabilities, alongside the metaFlye algorithm assembly. This approach aimed to uncover the organism's metabolic pathways and identify the genes accountable for polyhydroxyalkanoate (PHA) production.

Preliminary results: The exhaustive genome sequencing of strain B12 revealed a circular chromosome spanning 4.05 Mbp. Among the discerned genetic elements were those associated with PHA metabolism, carbon utilization, and energy production. These genetic signatures were then juxtaposed against analogous species' metabolic profiles, providing valuable insights. Detailed annotation of the identified genes demonstrated the presence of typical PHA biosynthesis-related genes such as phaA, phaB, phaE, and phaC.

Preliminary conclusions: This comprehensive evaluation facilitated an initial comprehension of their organizational framework. Furthermore, a comprehensive exploration identified regions potentially encoding proteins through a similarity search, ultimately yielding a comprehensive prediction of 5,290 genes.

Gabriel Liscia Catuzo
University of São Paulo

Abstract Title: CO2 hydrogenation to higher alcohols using K-promoted Cu-Fe/UiO-66 catalysts

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Abstract: Carbon dioxide is a greenhouse gas that plays a crucial role in climate change. In this way, the production of higher alcohols (HAs) from CO2 hydrogenation is a very attractive route for producing value-added compounds, and in addition, mitigating this pollutant. In this work, we synthesize,
characterize, and evaluate UiO-66 MOF-supported Cu-Fe catalysts in CO2 hydrogenation. Three catalysts were synthesized, containing Cu/Fe weight ratios equal to 1, 2, and 5. The Cu/Fe ratio was crucial in CO2 conversion and product distribution. The 15Cu15Fe-5K sample, with a Cu/Fe ratio equal to 1, containing a balanced proportion between Cu and Fe atoms, led to a higher yield for ethanol (2.1 molEtOH.kgcat 1.h-1, with CO2 conversion of 41.5%) due to its high basicity and good hydrogenation capacity, producing the two active species, *CO and *CHx, in abundance and in an excellent proportion, representing the highest C-C coupling capacity

Keywords: MOF UiO-66, Cu-Fe catalysts, CO2 hydrogenation, higher alcohols.

Introduction and Objectives: Higher alcohols synthesis from CO2 hydrogenation is a very promising alternative to transform CO2 into high-value products. However, a suitable higher alcohol synthesis (HAS) catalyst usually involves a striking balance between dissociative CO activation (alkylation) and non-dissociative CO activation (alcohol formation). One of the main challenges of this reaction is to convert the main intermediate, CO, into the desired products. Using CuFe-based catalysts, the Cu atoms activate the CO associatively, keeping it as the active specie *CO, while the Fe atoms dissociate it, transforming the CO into the *CHx active specie. The C-C coupling of these two species produces higher alcohols. In this way, the Cu/Fe ratio has been pointed out as crucial in CO2 conversion and product distribution. MOFs are a class of crystalline nanoporous materials that exhibit adaptability through large accessible surface areas. Furthermore, the pores can be functionalized through the addition of functional groups that favor the adsorption of gases, such as CO2. Furthermore, the synergistic effect between MOFs and functional materials can effectively improve the catalytic performance of these materials. To date, there are no Cu Fe-UiO-66-based catalysts that have evaluated the production of higher alcohols from the direct hydrogenation of CO2. In this sense, this work aims to obtain a new catalyst containing Cu and Fe supported on MOF UiO-66 for the production of higher alcohols through the catalytic conversion of CO2.

Methodology: 250-mL scintillation vial, 1,4-benzenedicarboxylic acid (500 mg) and zirconium tetrachloride (668 mg) were dissolved in a solution containing DMF (200 mL) and acetic acid (14 mL). The vial was sealed and heated in a 120 °C isothermal oven for a day. A white powder was collected by centrifugation (10,000 rpm, 7min), washed four times with DMF (20 mL × 4) over 24 h period, and four times with acetone (20 mL × 4) over a 24 h period. Finally, UiO-66 was dried under a dynamic vacuum overnight at room temperature and activated at 120 °C under vacuum for 24 h. The catalysts were prepared by incipient-wetness impregnation of aqueous solutions of copper, iron, and potassium precursors on the UiO-66.

The resulting precursors were dried at 90 ºC overnight and then calcined in N2 at 300 ºC for 3 h at a heating rate of 3 ºC min–1

Preliminary results: From the XRD patterns and N2 adsorptions/desorption isotherms of calcinated MOF UiO-66, the material has high crystallinity and B.E.T area that matches very well with data found in the literature. Furthermore, from TEM images, the crystals of this material have octahedral and intergrown morphology with well-defined faces and edges, similar to those reported by literature for UiO-66. After wet impregnation, the CuFeK/UiO-66 catalysts were analysed from several characterization techniques. The samples were labeled as xCuyFe-zK, where x, y, and z correspond to the element's loadings from EDS results. Three samples were synthesized, named 25Cu5Fe-5K, 20Cu10Fe-5K, and 15Cu15Fe-5K. The Cu/Fe ratio and the weight loadings of the metals are especially relevant parameters as they dictate the proportion between the two active phases (which have different catalytic properties) and the particle size. From TPD-H2 results, the H2 concentration increased considerably with the Fe content, since these atoms have a greater hydrogenation capacity in comparison with Cu. Analogous to TPD-H2, the number of basic sites, quantified from the TPD-CO2 technique, also increased with the Fe content. It is noteworthy to mention that K atoms are good donors of 4s electrons to carbon dioxide molecules, resulting in a lowering of the activation energy necessary for the hydrogenation of this reactant. It makes this element a very suitable promoter for this reaction. The catalysts were applied in this reaction. The 15Cu15Fe5K/UiO-66 sample achieved the best balance between dissociative and non-dissociative activation of CO, resulting in an optimized production of ethanol and higher alcohols (2.1 molEtOH.kgcat-1.h-1, with CO2 conversion of 41.5%). The results for TPD-CO2 and TPD-H2 show a good capacity to activate both reactants used in the reaction. The greater ethanol production for these samples shows that there is an increase in the non-dissociative adsorption of CO, provided by Fe species, which favors the *CHx - *CO coupling for the formation of this compound. The dissociation of this intermediate also justifies the lower selectivity towards CO. On the other hand, the Cu-rich sample, 25Cu5Fe-5K, led to a lower CO2 conversion (23.2%) and higher selectivity toward CO, showing a lower C-C coupling capacity, since the non-dissociative activation of *CO, provided by the Cu atoms, was predominant. CO2 hydrogenation was also accompanied by DRIFTS. The bands at 1464 and 1545 cm-1, more evident for the 15Cu15Fe-5K sample, refer to the *CH3COO species. The presence of these bands, added to the fact that *CO and *CHx were identified in the experiments, reinforces the theory of HAs formation from C-C coupling, in which CO, generated through r-WGS, is hydrogenated to CHx*, followed by *CHx - CO insertion.

Preliminary conclusions: Cu-Fe/K-UiO-66 catalysts were synthesized and characterized by some relevant techniques. The proportion between Cu and Fe particles supported on MOF UiO-66 proved to be fundamental in the conversion of CO2 and distribution of products, since an adequate balance between the hydrogenation capacity and activation of CO2 was fundamental in the formation of higher alcohols. The 15Cu15Fe-5K sample, with a balanced proportion between Cu and Fe atoms, led to a greater yield of higher alcohols due to its high basicity and

high hydrogenation capacity, producing the two active species *CO and *CHx , confirmed by DRIFTS analysis, in abundance and in an optimal proportion, favoring chain growth reactions.

Antonio Carlos Roveda Júnior
University of São Paulo - Instituto de Química de São Carlos

Abstract Title: Surface modification of copper electrodes for electrochemical CO2 reduction

Authors' Names & Affiliation Institutions of all authors (in order for publication): Antonio Carlos Roveda Júnior, Fabio Henrique Barros de Lima*

Abstract: The aim of this project is to produce metallic copper (Cu) electrodes coated with the polymer polybenzimidazole (PBI) for use in Electrochemical reduction of CO2 (ECO2RR). Following the chemical coordination of PBI on the Cu surface, we observed enhanced selectivity toward methane and ethylene as well as a decrease in the competitive hydrogen (H2) evolution.

Keywords: CO2 reduction, copper, surface modification, polybenzimidazole.

Introduction and Objectives: Copper (Cu) catalysts have shown the highest ability to produce hydrocarbons and alcohols such as ethylene and ethanol via Electrochemical Reduction of CO2 (ECO2RR). However, the development of systems capable of converting CO2 on an industrial scale into multicarbon compounds (C2+) employing electrocatalysts with high selectivity, stability, and Faradaic efficiency is still a long way off. One strategy in this approach is the covering of Cu electrodes with organic molecules. In general, the coating improves Faradaic efficiencies for C2+ products, reduces H2 generation, and improves catalyst stability when compared to the respective electrodes without the coating. Therefore, the aim of this project is to produce metallic copper (Cu) electrodes coated with the polymer polybenzimidazole (PBI) for use in Electrochemical reduction of CO2 (ECO2RR).

Methodology: The copper electrode is immersed in HNO3 (5 M) solution for 5 minutes, washed with water, dried in air, and then, reacted in a DFM solution of polybenzimidazole (0,03 %) at 50 °C for 15 minutes. Then, the copper electrodes are placed in a closed vial for drying. The electrochemical experiments were performed in a homemade H-type cell equipped with three electrodes. The cathode and anode were separated by a Nafion membrane. A platinum mesh was used as counter electrode, and a Ag/AgCl as a reference electrode. All reported potentials were converted to the reversible hydrogen electrode (RHE) scale. All working potentials were controlled with a Autolab Potentiostat (PGSTAT30) under room temperature.

The working electrolyte was an aqueous 0.1 M KHCO3 solution. Before every CO2 reduction experiment, CO2 was bubbled through the electrolyte for at least 45 min to obtain a CO2 saturated solution. The Ohmic resistance was evaluated by electrochemical impedance spectroscopy (EIS) at Open circuit potential (OCP), and 85% Ohmic drop compensation was applied to all subsequent experiments. Electrolysis was performed at fixed potentials for 60 min, constantly purging the electrolyte with CO2 at 10 mL/min for a stable pH and continuous CO2 supply. A gas sample was taken during 10 min in a gas sampling bag (Tedlar). Four samples for each potential taken (average and standard deviation). The gas products from CO2 reduction were analyzed using a Agilent 8860 GC system. The GC system was equipped with a FID, used to detect hydrocarbons, and a TCD for H2. The Faradic efficiencies (FE) were calculated by combining the electrochemical and GC data in using FE = (F × ne− × mol product / electrolysis charge), where F = Faraday constant and ne− = number of electrons necessary to generate each product.

Preliminary results: Copper-modified with PBI were characterized by Raman and nano-FTIR (s-SNOM) and the spectra have shown the characteristic bands of the PBI polymer. Scanning Electron Microscopy (SEM) revealed significant differences on the surface of the Cu electrode modified with PBI (CuPBI) in comparison with the pristine Cu. A homogeneous granular pattern was observed in the surface of CuPBI. S-SNOM experiments also revealed a homogeneous distribution of PBI over the surface of Cu. The Preliminaryy FE experiments revealed that H2 production was lower in CuPBI vs. Cu, and the production of CH4 and C2H4 was higher in CuPBI.

Preliminary conclusions: In summary, a methodology for producing copper electrodes coated with PBI was devised, and characterization results utilizing spectroscopic and microscopy techniques revealed that the copper surface was uniformly covered with PBI. According to the electrocatalysis results, Cu coated with PBI inhibited the H2 evolution while favoring the generation of methane and ethylene. Our findings contribute to a deeper understanding of ECO2RR activity and selectivity in PBI-modified Cu electrodes, and they demonstrate that coordination with functional molecules is a potential technique for developing selective, stable, scale-up catalysts.

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Abstract Title: Micractinium sp., mangroves, and biorefineries: A sustainable trio for third-generation ethanol

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Abstract: Global population growth and modern lifestyles have heightened the worldwide energy demand. Fossil fuels are crucial in meeting this demand, accounting for approximately 80%. However, the indiscriminate use of these resources has adverse implications, particularly concerning CO2 emissions, which play a pivotal role in climate change. In this context, the transportation sector is a significant contributor to emissions. Therefore, to address this pressing challenge and align with the United Nations' Sustainable Development Goals (SDG), it is imperative to seek low-carbon alternatives, such as ethanol derived from sugarcane and corn. However, these biomasses face critical dilemmas, such as competition between food and fuel production. Third-generation ethanol (3G) from microalgae biomass emerges as a potential solution. These microorganisms can convert light, CO2, water, and nutrients into biomass, glucose, and O2, demonstrating the capacity to accumulate substantial amounts of carbohydrates, which can be hydrolysed and fermented to produce ethanol. However, the production of 3G ethanol faces significant challenges. In this regard, strain selection is the most critical step for successful 3G ethanol production, requiring productive and adaptable strains under different environmental conditions. Furthermore, using microalgae to produce other high-value bioproducts is essential for 3G ethanol success. In this context, strains isolated from mangroves show promise due to their adaptability and resilience, although their biotechnological potential is still underestimated. This work reports a strain identified as Micractinium sp. B5, isolated from the Baixada Santista mangrove (SP, Brazil), shows high biotechnological potential. Strain B5 was cultivated in a complete nutrient culture medium, and after cellular growth, it was subjected to nitrogen deprivation to stimulate bioproduct accumulation. The cultivation process lasted 14 days, consistently under 5% CO2 (v/v). The obtained biomass was used to determine the cell's biochemical composition. In addition, the acid hydrolysis conditions were optimized to obtain monosaccharides for subsequent alcoholic fermentation using S. cerevisiae. Micractinium sp. B5's biochemical composition comprised approximately (w/w) 30% total carbohydrates, with about 23% corresponding to glucose and

24% lipids, notably producing C18 fatty acids with high added value. Monosaccharides obtained after chemical hydrolysis, under optimized conditions, were converted into ethanol with a yield exceeding 80% compared to the theoretical maximum. Furthermore, the obtained hydrolysate proved to be free of potentially inhibitory substances for alcoholic fermentation, producing only low concentrations of acetic acid. The results show that strain B5 has high potential for the viable production of 3G ethanol and aligns with the biorefinery concept. Besides, it represents a promising biomass contribution to achieving various SDGs.

Keywords: Microalgae; Energy transition; Mangrove forest; CO2 mitigation.

Introduction and Objectives: Global population growth and modern lifestyles have heightened the worldwide energy demand. Fossil fuels are crucial in meeting this demand, accounting for approximately 80%. However, the indiscriminate use of these resources has adverse implications, particularly concerning CO2 emissions, which play a pivotal role in climate change. In this context, the transportation sector is a significant contributor to emissions. Therefore, to address this pressing challenge and align with the United Nations' Sustainable Development Goals (SDG), it is imperative to seek low-carbon alternatives, such as ethanol derived from sugarcane and corn. However, these biomasses face critical dilemmas, such as competition between food and fuel production. Third-generation ethanol (3G) from microalgae biomass emerges as a potential solution. These microorganisms can convert light, CO2, water, and nutrients into biomass, glucose, and O2, demonstrating the capacity to accumulate substantial amounts of carbohydrates, which can be hydrolysed and fermented to produce ethanol. However, the production of 3G ethanol faces significant challenges. In this regard, strain selection is the most critical step for successful 3G ethanol production, requiring productive and adaptable strains under different environmental conditions. Furthermore, using microalgae to produce other high-value bioproducts is essential for 3G ethanol success. In this context, strains isolated from mangroves show promise due to their adaptability and resilience, although their biotechnological potential is still underestimated. This work reports a strain identified as Micractinium sp. B5, isolated from the Baixada Santista mangrove (SP, Brazil), shows high biotechnological potential.

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Preliminary conclusions: The results show that strain B5 has high potential for the viable production of 3G ethanol and aligns with the biorefinery concept. Besides, it represents a promising biomass contribution to achieving various SDGs.

Aluizio Jose Salvador
University of São Paulo

Abstract Title : Development of a microfluidic device (rock on a chip) compatible with synchrotron techniques for in-situ monitoring of CO2 storage by rocks

Authors' Names & Affiliation Institutions of all authors: Aluizio Jose Salvador (USP/CNPEM), Nathaly Lopes Archilha (CNPEM), Caetano Rodrigues Miranda (USP)

Abstract: This work is one of the branches of an interdisciplinary collaboration, that seeks to understand the rates and mechanisms of key geological reactions and their impact on geological sequestration in the Rio Bonito formation. This comprises controlled mineralization experiments and in-depth characterization of products of mineralization on formation rocks. In this proposal, samples from prospects and outcrops near the Rio Bonito formation and plugs extracted directly from the potential reservoir will be analyzed. Data from dissolution mechanisms with weak acids are presented and will provide experimental validation of previously established atomistic models, and finally help to understand the mineralization mechanisms activated during laboratory tests.

Keywords: carbon dioxide, mineral sequestration, microfluidic.

Introduction and Objectives: Microfluidic devices have emerged as an essential tool for reproducing large scale's phenomena in a controlled environment. Their main characteristics are the reduced size, low weight, and high throughput, as well as the capacity of operating with small amounts of samples through micrometer and/or sub-micrometer channels. In this sense, devices for reproducing flow in simplified pore structures have been fabricated using engineered materials such as silicon, glass and PDMS. However, these devices present inherent limitations once they do not fully reproduce complex micropores structures and do not replicate the natural chemical reactivity of the real rock surface. As a result, these micromodels do not

fully evaluate the fundamental mechanisms of flow, transport, and reactions within the context of an actual reservoir.

Methodology: overcome these limitations, it was developed a microfluidic device using a real rock as the sample. The device was projected to be characterized at the Carnaúba beamline of the Brazilian Synchrotron Light Laboratory, aiming at in-situ monitoring the potential of rocks from the Rio Bonito formation in capture and store carbon dioxide. In one of the surfaces (front face) of a slice 5 mm thick, a channel of 1 mm wide, 0.5 mm deep, and 10 mm long was drilled with two holes at the ends point along the rock. A Kapton tape was used to seal the channel in the front face and keep the fluid flow only inside it. The holes connect both surfaces of the slice and serve as the fluid inlet and outlet, in which a flux in the channel can be set out with a peristaltic pump. Hydrochloric and Carbonic acid solutions were injected into the channel during ten days, to initially evaluate the dissolution and precipitation mechanisms. The process was evaluated by performing 2D images using a contrast of X-ray fluorescence and punctual X ray absorption measurements in specific atoms.

Preliminary results: Using ambient conditions of temperature and pressure it was not observed any mineral precipitation along the channel. However, these first tests using this novel and original Rock on a Chip device were important for its validation. The considered parameters such the shape and sealing of the channel, were found to be optimal for the intended experiments. No leaks were observed during the runs and all intended measurements were conducted without issues. Moreover, important chemical information was obtained through X-ray fluorescence maps, which will help and guide us in future experiments. In addition, the X-ray absorption measurements showed the microstructural changes occurring in the samples submitted to the mineralization experiments. The interpretation and complete understanding of all these spectra is in progress.

Preliminary conclusions: This set of data was important to validate the device, however, some improvements are going to be made to increase the chances of observe the mineral precipitation. The main point is considering pressure along the channel, which is a fundamental parameter of the CO2 capture and storage. This phase is yet being planned, but it is intended to insert the rock into a PDMS box, complete sealed that will allow inject a pressurized solution. Meanwhile, the actual device will be used to better investigate the mineral dissolution by considering different acid solution in different concentrations. To understand the mineral dissolution rates is fundamental to know what will be the results from the CO2 interaction.

Natalia Lima Vergilio
Unicamp

Abstract Title: Geochemical Modeling of Alteration in Pre-Salt Carbonate Reservoir Rocks In Response To CO2 Injection

Authors' Names & Affiliation Institutions of all authors (in order for publication): Lima-Vergilio, N; De-Campos, AB (Unicamp & Unicamp).

Abstract: Oil extraction is one of the main sources of carbon dioxide. An alternative to burning the gas that is extracted along with the oil is to use it as an EOR and CCUS method in siliciclastic and carbonate reservoirs, the latter being geochemically reactive and can trigger changes in the reservoir. Geochemical modelling has been used in recent years to predict scenarios of changes in reservoir rocks when gas is injected. Although it is a relevant topic, there are currently few published studies on changes in the geological properties that can occur in Presalt carbonate reservoir rocks in response to long-term CO2 injection, considering that gas injection is a reality in the Presalt. Taking into account this scenario and the economic relevance of the Santos Basin Presalt, a 1D reactive transport geochemical model was proposed for the 20 years of continuous carbonate brine injection, to understand how CO2-fluid-rock interaction occurs in the long term. Various customizations were also proposed for the Phreeqc program to adapt it to the conditions found at Presalt. The modelling was carried out to compare points at different distances from the injection well, modelling with different levels of refinement and the total carbon accumulated over the proposed 20-year period. Among the main results found are: 1) equilibrium was not reached for the larger minerals in the vicinity of the injection well at the end of the period; 2) the pH stabilized at around 7.45; 3) the total accumulated carbon calculated was 25.5 m^3/kg of rock in the vicinity of the injection well; 4) the customization and refinement of the geochemical modelling significantly alters the final results.

Keywords: CCUS, Geochemical Modelling, Reactive Transport, Phreeqc, Presalt, Santos Basin.

Introduction and Objectives: CO2 is currently considered to be the main cause of the greenhouse effect (Metz et al., 2005), a problem that is also related to the hydrocarbon production chain since this activity produces a large amount of gas. An alternative to mitigate the adverse effects of CO2 production in oil wells and its emission into the atmosphere is to inject the gas into carbonate reservoirs as an EOR and CCUS method (Emberley et al., 2004; Cantucci et al., 2009; Romero & Pereira, 2014; Rosa et al., 2016; Siqueira et al., 2017). Several geochemical processes occur in carbonate reservoirs when CO2 is injected, however, the dynamics of the geochemical processes and their consequences in geological, physical, and chemical terms for the reservoir rocks are still little known, and this is a relevant topic for research in the oil area, since the reinjection of CO2 into offshore basins is a reality in the

country. Despite the relevance of the topic, no studies have been found in the current literature on long-term geochemical modelling of the effects of this injection, which would be useful for predicting the behaviour of carbonate reservoir rocks in the face of gas injection.
This research aimed to improve geochemical modelling to generate more reliable alteration

scenarios in the carbonate reservoir rocks of the Santos Basin Presalt in response to CO2 injection.

Methodology: The model was developed using data from well 9-BRSA-716-RJS, located in the Tupi Field, provided by the ANP's Exploration and Production Database, which was added to the geochemical modelling program Phreeqc. 1D reactive transport modelling was carried out for 5 different distances from the injection well in 100 stages, totalling 20 years of injection. The customization of the geochemical modelling included a new database for the pressure and temperature conditions of the Presalt, and kinetic rates for all minerals, trace minerals, and secondary minerals.

Preliminary results: In the modelling, equilibrium was reached for most of the minerals, and the pH at the points furthest from the injection was well, within the 20-year interval. In the vicinity of the injection well, all the larger minerals continued to precipitate or dissolve until the end of the proposed period, establishing a buffer effect that allowed the pH to remain balanced. Some minerals, such as talc, anhydrite, dawsonite, and cristobalite, dissolved completely, proving not to be stable under gas injection conditions. Most of the interactions took place in the first few years and were more intense in the vicinity of the injection well. A comparison of the tests generated with different levels of enhancement showed that the inclusion of trace minerals interferes directly and significantly with the final results and the evolution of mineral concentration.
The total carbon stock was also calculated, with 80% of the total being structurally trapped, 2% dissolved/residual, and 18% mineralized, at the end of the proposed 20 years. Comparing distances, there are 25.5 kg/m³ rock (near the injection well), 12.06 kg/m³ rock (halfway between the wells), and 12.06 kg/m³ rock (near the producer well).

Preliminary conclusions: The unpublished results of this research may help in the development of more accurate geochemical modelling inside and outside academia, and increase understanding of the geochemical and mineralogical response of carbonate rocks to CO2 injection under reservoir conditions in the Santos Basin Presalt.

Paulo Henrique dos Santos Santana
University of São Paulo

Abstract Title: Stability of turbulent oxy-methane flames in an internal recirculation combustion chamber

Authors' Names & Affiliation Institutions of all authors:
Paulo Henrique dos Santos Santana (University of São Paulo), Helio Henrique Santomo Villanueva (University of São Paulo) e Guenther Carlos Krieger Filho (University of São Paulo)

Abstract: This work assesses the effect of dilution on three turbulent oxy-methane flames diluted with CO2 in an internal recirculation combustion chamber. The anchored, lifted, and MILD flames were established keeping the bulk velocity of O2 + CO2 fixed at 30 m/s, changing the mole fraction of CO2 (0% − 72%) and the equivalence ratio (0.5 − 1.0). From the measurement of the OH∗ radical emissions by chemiluminescence, the mean fields indicated the flames topology and standard deviation the emissions fluctuation. The anchored flame possessed the jet shape and was established at lower dilutions, the lifted flame was shown to produce great noise linked to liftoff height, whereas the MILD/flameless regime was evenly distributed in the chamber. The blowoff occurred at a constant laminar flame velocity by varying the equivalence ratio. This result indicates that the laminar flame velocity better represents the blowoff phenomenon than the adiabatic flame temperature.

Keywords: Oxy-combustion, flame stability, chemiluminescence, combustion regimes, blowoff.

Introduction and Objectives: In the context of Carbon Capture Utilization and Storage (CCUS) technologies applications, oxy-fuel combustion appears as a promising route to reduce carbon dioxide emissions. In oxy-fuel combustion nitrogen is not present, or is present in a small amount, consequently the temperature of the combustion gases is little diluted and becomes much higher than in the air-fuel case. However, in power plant applications, the high temperature at the turbine inlet is an obstacle. Therefore, it is essential to use a substance to replace nitrogen as a temperature diluent. The immediate candidates to dilute the temperature are carbon dioxide and water vapour, which can be recycled from flue gases. In this way, the high concentrations of CO2 and H2O in the combustion gases facilitate the separation and capture of carbon dioxide. Despite this, the energy cost of O2 forces combustion with oxygen close to stoichiometry, which makes it essential to perform combustion in an increasingly efficient manner. Added to this, the different thermophysical and thermochemical properties of CO2 and H2O, compared to N2, change the flame stability characteristics. This study investigates the effect of CO2 dilution on flame stability of a non-premixed turbulent oxy-fuel configuration in an internal recirculation combustion chamber. OH∗ chemiluminescence

distributions were used to determine the operation range of different combustion regimes and the stability of the combustion chamber based on the blowoff analysis.

Methodology: The combustion chamber was developed at Instituto Superior Técnico (IST) to operate stably in the conventional flame and MILD/flameless regimes in air-fuel combustion. The chamber consists of a quartz tube 100 mm in diameter and 350 mm in length resting on the burner and fixed by an upper flange. The quartz tube was wrapped in three layers of alumina ceramic blanket, each layer with 20 mm, in order to achieve thermal insulation with the laboratory environment. The oxidant (O2) and the diluent (CO2) are pre-mixed before being inserted into the burner; this mixture enters the chamber through a 10 mm centred on the burner. The fuel (CH4) is inserted into the burner through 16 holes of 2 mm in diameter equally displaced 15 mm from the centre of the burner. Thus, the methane and the O2/CO2 mixture mix only inside the combustion chamber, constituting a non-premixed configuration. The $OH*$

radical chemiluminescence measurement system was set up with a 306.6 ± 1.5 nm bandpass filter connected to an objective lens with UV limits between 250 nm and 410 nm, focal length 100 mm f/2.8 from CERCO model 2073. This set was coupled to a C10880 Hamamatsu Photonics K.K. image intensifier and a 12-bit CMOS camera with a sensor array of 1280×800 pixels and 20 μm of pixel pitch (V311 - Vision Research Inc.). A 575-8C pulse generator from Berkeley Nucleonics Corporation synchronized the camera and image intensifier and was controlled by the Dynamic Studio software from Dantec Dynamics A/S. In each measurement, 17375 images were acquired at a rate of 2 kHz. To adapt this acquisition frequency, 960 × 512 pixels of the sensor were used. All measurements were carried out keeping the bulk velocity constant, thus maintaining the so-called similar cold-flow conditions, in order to maintain close turbulent intensities in the comparison between flames. The flow rates of O2 and CO2 were adjusted to maintain the velocity at 30 m/s in the burner's center jet. The methane flow was controlled in such a way that the equivalence ratio was unity, in the case of chemiluminescence measurements, or lean in blowoff measurements. The blowoff measurements were performed first keeping the thermal power fixed and the oxygen flow sufficient to reach 30 m/s in the central jet. From there, the flow rate of O2 was decreased and that of CO2 increased slowly, in such a way that the bulk velocity remained constant until the blowoff event. During the operation, the flame regimes changed from the anchored flame to the lifted flame, in some cases reaching the MILD/flameless regime and finally the blowoff.

Preliminary results:

Anchored Flames

The anchored flames always maintained the well-known jet topology attached to the central edge of the burner outlet. In the mean field, maximum intensity values are seen at the jet boundary. Boundary, in which the greatest intensity gradients occur when analyzed in the radial direction. Values in the standard deviation field define three regions: inside, boundary, and outside the jet. There is a pronounced definition of the jet boundary with maximum values. This occurs similarly to large turbulence scales, at the jet boundary, where the maximum gradients

occur, the most significant fluctuations and consequently the highest turbulent kinetic energy.

Lifted Flames

The lifted flames produced loud noise linked to the height oscillation and the shape of the flame. This occurred in the range from 3726 K to 2795 K of Tad. The maximum mean intensity of the lifted flame was centered in the measurement window above 150 mm. The intensity decreased with a smoother gradient than seen in the anchored flame. In addition, the oscillations make the distribution asymmetrical. The intensity standard deviation field shows peaks distributed at the bottom of the flame indicating liftoff height variability.

MILD/Flameless Regime

In the flameless regime the noise decreases drastically in relation to the lifted flame noise. In addition, the luminosity was uniform inside the chamber with a reddish color. The emission peaks of OH∗ reduced from 564 a.u., to 361 a.u. and 94 a.u. for the anchored, lifted, and

flameless, respectively. This reduction in intensity indicates that reactions occur at a lower intensity in this regime, although chemical reactions are still present, since the noise peak intensity observed with the camera shutter closed is 90 a.u.. The mean and root mean square fields confirm the uniform distribution of combustion in the chamber. On average, there is a slight increase above 150 mm only on one side of the radial positions, which points to an unexpected asymmetry, which is also observed in the root mean square field.

Blowoff Analysis

The blowoff procedure was applied to a series of six thermal powers, in which the blowoff occurred in different equivalence ratios. It can be seen that the adiabatic flame temperature at blowoff decreases with the equivalence ratio and the thermal power from 2182 K to 1856 K. The laminar flame velocity varies between 13 cm/s and 15 cm/s, with a mean value of 13.9 cm/s. Therefore, there is a correlation between the blowoff phenomenon and the global laminar flame speed, which was calculated with the input parameters. These results are related to keeping the bulk velocity constant at the inlet, which means that it is assumed that ultimately the turbulence time scales were kept in the same order of magnitude. Thus, increasing diluent alters chemical kinetics and transport properties in such a way that ultimately increases the characteristic chemical time scale until blowoff occurs.

Preliminary conclusions: In this paper, the effect of CO2 dilution on the flame stability of a non-premixed turbulent oxy-methane configuration in an internal recirculation chamber at atmospheric pressure was presented. The operational conditions were set keeping the bulk velocity of the O2/CO2 mixture fixed and the anchored, lifted, and MILD/flameless regimes were observed until blowoff. OH∗ chemiluminescence measurements showed the mean topology of the flames, in addition to providing an indication of turbulence by the standard deviation field. The anchored flame exhibited a well-defined jet structure stabilized in the

combustion chamber inlet plane. The lifted flame produced great noise and oscillations in shape and liftoff height. In the MILD/flameless regime, the reactions were more uniformly distributed inside the chamber and presented a considerable reduction of OH∗ and noise emissions. The blowoff was studied in the equivalence ratio range from 0.5 to 1.0. The results indicate that the blowoff occurs at a constant laminar flame velocity regardless of the equivalence ratio. Although the chamber configuration is non-premixed, this correlation suggests that the laminar flame velocity is the representative parameter of the characteristic chemical time scale changes in the flame caused by dilution.

Pedro Henrique de Paula Sabanay
Universidade de São Paulo

Abstract Title : A spectroscopic study of Superbase-based Deep Eutectic Solvents for CO2 Capture

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Abstract: The growing demand for viable methodologies for capturing CO2 has led to the emergence of various liquid and solid materials that are easy to prepare, inexpensive, recyclable, and environmentally friendly. In this context, a new class of solvents known as deep eutectic solvents (DES) has gained prominence due to their advantageous properties. This project aims to evaluate the CO2 absorption capacity of different DES through the combination of various spectroscopic measurement methods for material and product characterization. DES were prepared in different proportions from superbases, alkanolamines, and urea derivatives. CO2 absorption was conducted at different pressures at a constant temperature, using vibrational spectroscopy techniques (Raman and IR) to characterize the DES in the absence and presence of the gas. Through this study, it was found that DES formed from superbases and amines are promising CO2 fixatives with high sorption capacities, while DES formed from urea derivatives have reversely absorbed CO2 driven by strong interactions. However, further studies are needed for a complete understanding of this process. The results demonstrate the potential of deep eutectic solvents formed from superbases in capturing carbon dioxide. By analyzing spectroscopic results, a better understanding of the mechanisms involved in the gas sorption process in these solvents can be gained. Consequently, in the future, it will be possible to evaluate the possibility of converting the gas into value-added materials and optimize gas capture with more specific DES.

Keywords: carbon dioxide, DES, vibrational spectroscopy.

Introduction and Objectives: The emission of carbon dioxide (CO2) and another greenhouse gases (GHGs) have gradually increased over the years, resulting in various environmental impacts. It reached its peak in May 2020 when atmospheric CO2 levels reached 413 ppm. Therefore, the optimization of CO2 capture is urgently needed. Currently, the commonly used method for CO2 capture in the industry involves a 30% aqueous solution of monoethanolamine (MEA), widely commercialized due to its efficiency and reversibility. However, this technique has several problems such as the volatility of the amine, toxicity, low thermal stability, and high energy requirements for recovering captured CO2, making the search for new technologies extremely important. To improve this process, a new class of solvents has been studied for capturing these compounds. Thus, a recent class of deep eutectic solvents (DES) has gained prominence due to their properties such as ease of preparation, low production cost, greater biodegradability, and lower toxicity. Typically, DES are composed of two chemical species, a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD). The numerous possible combinations of HBAs and HBDs allow for the preparation of DES with desirable properties.

It is known in the literature that basic functional groups in solvents favor CO2 sorption due to the nature of CO2. Therefore, highly basic and unstable compounds in their pure form, known as superbases, have been used to obtain functionalized DES for efficient CO2 capture. The investigation of HBA-HBD and DES-CO2 interactions is the key point for a fundamental understanding of the CO2 capture and conversion process. Therefore, this project employed vibrational spectroscopy (Raman and IR) and CO2 sorption measurements as a function of pressure and temperature to investigate interactions in DES and their mixtures with CO2. A systematic study of superbases-based DES for CO2 capture was conducted, both from a fundamental perspective, involving spectroscopic and thermodynamic characterization of interactions, and from a practical perspective, evaluating absorption capacity and the possibility of conversion into higher-value products.

Methodology: Different deep eutectic solvents (DES) were tested, prepared in various proportions of donors and acceptors using superbases as HBAs and urea derivatives and amines as HBDs. The characterization of the solvents was carried out both in the presence and absence of CO2 using vibrational spectroscopy (Raman and IR). The DES were prepared following adaptations from methods described in the literature. For mixtures containing amines, the preparations were carried out in an inert atmosphere with magnetic stirring for 1 hour and kept closed until complete homogenization. For mixtures prepared with urea derivatives, the system was heated to 40°C, stirred for 1 hour, and kept closed until complete homogenization. Two CO2 absorption measurements were conducted. In the first measurement, an aliquot of the DES synthesized in the previous steps was used for the gas absorption experiment. It was transferred to a two-neck flask and maintained under a constant gas flow with magnetic stirring for 30 minutes at a temperature of 35-40°C controlled by a silicone oil bath. The system was sealed with an oil seal to prevent contact with the atmosphere. For the mixture of superbases with

amines, an additional measurement was performed using the magnetic suspension microbalance, which allows measuring CO2 absorption by varying gas temperature and pressure. The determination of CO2 solubility was carried out by saturating the gas in the DES at different pressures and a fixed temperature of 40°C in the pressure range of 0-25 bar.

Preliminary results: Analysing the infrared (IR) spectra of the mixtures revealed shifts and changes in the intensity of bands due to the presence of other functional groups and intermolecular interactions. These band changes indicate the formation of new interactions in the mixtures, such as hydrogen bonds, enabling the understanding of the mixtures as DES. Superbases exhibited a higher CO2 absorption capacity compared to amines and urea because they can reach equimolar absorption values, although the experiments did not replicate theoretical values due to the gradual increase in the viscosity of the mixture during the process. Mixtures based on superbases and amine derivatives in the ratio of 2HDA-1HBD have exceeded theoretical absorption values. However, mixtures of superbases with urea derivatives exhibited lower absorption capacities due to the formation of competitive hydrogen bonds for CO2 binding sites. The CO2 absorption capacity depends on intermolecular interactions among the components of the DES and the gas, especially DES-H2O interactions. As the formation of carbamate salt resulting from the CO2-amine interaction increased in the system, there was competition for the N-H bond responsible for carbamate formation, as this bond also formed hydrogen bonds with the salt.

Preliminary conclusions: The mixture of superbase and amines has proven advantageous for CO2 capture, resulting in a low viscosity liquid with two reactive components towards the gas. Mixtures formed with superbase and urea derivatives have shown promising results in CO2 capture. The IR characterization of the mixtures and the reactions products allowed the confirmation of absorptions mechanisms. In the next step, it is intended to conduct a deeper study on the physical and thermodynamic properties in this process in order to evaluate the real potentiality of those mixtures to CO2 capture.

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Abstract Title: Contributions to the lifetime widening of ZSM-5 zeolites in the ETH reaction

Authors' Names & Affiliation Institutions of all authors: Catalysis Group, Institute of Chemistry, UNESP – Araraquara.

Abstract: In this work we demonstrate that the generation of mesopores in ZSM-5 zeolite is an efficient strategy to extend propylene production by ethanol conversion. The benefit of

mesopore system is to avoid coke accumulation in the catalyst, thus reducing the pore blockage and deactivation. Moreover, by using CO2 as auxiliary gas in the reaction, propylene production is favoured.

Keywords: ethanol, propene, zeolite.

Introduction and Objectives: Ethanol to hydrocarbons (ETH) reactions have received special attention due to the environmental problems caused by using fossil fuels. Its potential can be especially explored in the brazilian scenario, where the production of ethanol from renewable sources is consolidated. These reactions can be catalyzed by protonic zeolites, especially H-ZSM-5, where the confinement effect is a key factor to produce C3+ hydrocarbons. However, the formation of active aromatic species on confined acidic sites results in the production of coke, deactivating the catalyst, which can be minimized using hierarchical zeolites, which contain meso and/or macropores, enhancing the diffusion of intermediate species and reaction products. The engineering of the pores of H-ZSM-5 zeolites, through post-synthesis treatment and in situ generation of mesopores and the control of their crystal size through the preparation of nanozeolites are addressed in this project. The optimization of the reactor operating conditions by using CO2 as auxiliary gas as well as the advanced characterization of the coke formed and its structural effects on the different zeolites will bring contributions that will allow optimizing the catalytic performance in the ETH reaction, by widening the lifetime of the catalysts.

Methodology: Conventional purely microporous ZSM-5 zeolite (MFI topology) was synthesized by a method previously reported by our group. The pristine sample was treated with NaOH to promote silicon removal and mesopore generation. The conditions for this treatment were optimized in order to preserve import characteristics of conventional zeolite (crystallinity, chemical composition and microporosity). Samples were characterized by XRD diffraction, nitrogen physisorption, EDS, thermogravimetry and FTIR with chemisorbed pyridine. The catalytic tests were performed at ambient pressure in a PID reactor operating at 450 C with ethanol flow of 0,05 mL/min and auxilary gas N2 or CO2 at 20 mL/min.

Preliminary results: By adjusting the NaOH treatment conditions for the desilication of ZSM-5, it was possible to prepare a sample with mesopores of around 10 nm in diameter, preserving the micropore volume (0.14 cm^3/g), crystallinity (100%) and o Si/Al (20). It was also observed that hierarchical zeolites present more accessible acid sites for chemisorption of pyridine as a probe molecule.
The hierarchical ZSM-5 was more stable in converting ethanol to propylene in terms of propylene selectivity. The pure sample (purely microporous ZSM-5) is deactivated within 24 hours, as the mesoporous ZSM-5 still produces propylene and ethene. The results of thermogravimetry of spent zeolites allowed us to conclude that the greater stability of the hierarchical structure is due to the low formation of coke, thus reducing deactivation due to pore obstruction.

Regarding the use of carbon dioxide as an auxiliary gas, the results showed that this mild oxidizing gas promotes the formation of propylene for a longer time. The role of CO2 is still under investigation.

Preliminary conclusions: The generation of mesopores in conventional purely microporous ZSM-5 zeolite is an efficient strategy to enhance propene production from ethanol, due to the low deactivation by coking. Moreover, carbon dioxide promotes the formation of propene for longer.

0811 - PS10 (TV3)

Chairs: Maurício Salles – Renato Monaro

Clarification notice: The majority of the pieces on display in this thematic track are the outcome of TotalEnergies-sponsored research.

Beethoven Narváez-Romo
University of São Paulo

Abstract Title: Carbon Emission Reductions in The University of Sao Paulo's Transportation

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2 University of Sao Paulo, Bioenergy Research Group – GBio, Av. Professor Luciano Gualberto, 1289, Sao Paulo-SP, Brazil.

Abstract: This work aims to estimate and compare emission reductions achievable through the implementation of renewable hydrogen vehicles in the transport sector at the University of São Paulo. As a methodological approach, carbon-neutral hydrogen production using the ethanol steam reforming route is considered, wherein energy and mass balances are carried out throughout the hydrogen chain. A baseline scenario for CO2 emissions is defined, taking into account the transport specifics: routines, frequencies, distances, and embedded technologies, along with their respective consumption coefficients. Subsequently, a comparative assessment is performed between renewable hydrogen technologies and the established baseline scenario. Results showed that replacing the current fleet of conventional internal combustion engine

buses with hydrogen-based options leads to a significant reduction in CO2 emissions per year, decreasing from 3185 to 874 tonnes CO2eq.

Keywords: Hydrogen, Decarbonization, CO2 emissions, Ethanol.

Introduction and Objectives: This work aims to estimate and compare emission reductions achievable through the implementation of renewable hydrogen vehicles in the transport sector at the University of São Paulo.

Methodology: As a methodological approach, carbon-neutral hydrogen production using the ethanol steam reforming route is considered, wherein energy and mass balances are carried out throughout the hydrogen chain. A baseline scenario for CO2 emissions is defined, taking into account the transport specifics: routines, frequencies, distances, and embedded technologies, along with their respective consumption coefficients.

Preliminary results: Results showed that replacing the current fleet of conventional internal combustion engine buses with hydrogen-based options leads to a significant reduction in CO2 emissions per year, decreasing from 3185 to 874 tonnes CO2eq.

Preliminary conclusions: Hydrogen-powered vehicles, despite being in development, offer a promising solution for decarbonizing the challenging transportation sector, thanks to zero emissions, long range, and potential in heavy-duty transport. Their success depends on addressing production methods, infrastructure, and utilizing green hydrogen sources.

Felipe Moreira Sallazar
Federal University of São Carlos

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: UAV-Assisted Fault Detection in Electrical Distribution Systems: Computational Simulation

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Abstract: Power transmission lines connected to wind farms are subject to the occurrence of short circuits that can leave the wind turbines unavailable for long periods of time, due to difficulties for the maintenance team in locating the exact location of the fault. Furthermore, these feeders can cross difficult-to-access regions, imposing additional difficulties on the maintenance team. Once the fault is located by an intelligent fault diagnosis system (detection, classification and location), an aerial drone will be activated to sense the environment at the exact fault location, reporting to the maintenance team for the correct planning of defect correction in medium voltage overhead feeders. This research aims to develop a 3D simulation environment for a wind farm to study the location of faults in medium voltage overhead feeders. In the environment, medium voltage overhead feeders and their surroundings will be simulated. A simulation of the drone that will carry out the inspection will also be carried out. In the simulation, the drone must be equipped with RGB and thermal cameras and 3D LiDAR. Furthermore, the simulation must be compatible with the ROS SDK of the M350 drone.

Keywords: UAV Path Planning; Defect Detection; Transmission Line Fault Detection; Gazebo; ROS; Computational Simulation.

Introduction and Objectives: An important research front for locating faults in wind farms is the integration of aerial drones into the fault diagnosis system. These drones will be activated automatically when a fault is detected in a medium voltage overhead feeder and, using specialized navigation algorithms, will proceed autonomously (without operator control) to the indicated location of the fault. The main objective of this project is the development of a 3D simulation environment for a wind farm. In this environment, mainly medium voltage overhead feeders and their surroundings will be simulated. The drone that will be used for the inspection will also be simulated, this drone will be equipped with RGB and thermal cameras and 3D LiDAR.

Methodology: We will utilize ROS and Gazebo software to construct a 3D simulator encompassing the wind farm, medium voltage feeders, and the drone. ROS (Robot Operating System) is a set of software libraries and open-source tools to assist in the creation of robot applications and which will be used to implement the drone's navigation algorithm and interfacing with sensors and cameras. Gazebo is a 3D graphical simulation software with integration with ROS that will be used to develop an environment representative of the wind farm with its medium voltage aerial feeders, which will be used in tests to simulate both the drone and its sensors and cameras inside of a virtual environment. In addition, the ROS will be

interfaced with the Onboard Software Development Kit (OSDK) of the DJI M350 drone so that the drone simulator is compatible with the real drone.

Preliminary results: s this work is currently underway, we have not yet obtained any results.

Preliminary conclusions: As this work is currently underway, we have not reached any conclusions yet.

Gabriel de Castro Biage
Universidade de São Paulo

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Cable Parameter Calculation Through the Finite Element Method

Authors' Names & Affiliation Institutions of all authors *Gabriel de Castro Biage (USP), Rooney Ribeiro Albuquerque Coelho (USP), Mario Leite Pereira Filho (IPT).

Abstract: For either overhead transmission line and subsea transmission line, the parameters of the line cable are input parameters for the existing transmission line models. As determining line parameters becomes an essential task, a literature review on the calculation of the line parameters using Finite Element Method was done. The methods studied were then validated from existing numerical and analytical results. All the methods implemented showed acceptable results when compared to the existing results in literature, but it neglects the proximity effect between conductors. It is needed to analyze the consequence of the proximity effect in subsea transmission lines and the environment return impedance in the calculation of cable parameters.

Keywords: Finite element methods, Power cables, Electrostatics, Magnetodynamics, Skin effect, Conducting materials, Dielectric materials, Frequency, Proximity effect, Cables, capacitance, electric resistance, electromagnetic fields, finite element analysis, Inductance, transmission line theory, umbilical cable.

Introduction and Objectives: For either overhead transmission line and subsea transmission line, the parameters of the line cable are input parameters for the existing models. This is true for models that represent the electrical quantities of the power line in the frequency domain and in the time domain. For this reason, determining line parameters becomes an essential task in

transmission line modelling. Several approaches to determine parameters analytically and numerically have been developed in this context. Analytical calculation methods were developed mainly for simplified geometries and, although there are correction factors that describe the variation of the parameters as a function of frequency, they do not always accurately model this phenomenon and are not applicable to all cases. From this point of view, the finite element method presents itself as an efficient tool for calculating transmission line cable parameters with high precision and ease of use. To calculate the parameters using the finite element method (FEM), the electromagnetic fields profile are initially calculated using the FEM, then the parameters are obtained from the field solution. The objective of this work is to study the existing methods in the literature for calculating cable parameters, evaluate their limitations and analyse them in the context of subsea umbilical cable.

Methodology: To carry out the activities foreseen in the scope of the project, four main work fronts can be highlighted: i) Study and description of the cable parameters used in transmission line models ii) Study of the methodology and procedure for calculating the parameters through the FEM iii) Implementation and automation of the calculation routine using commercial finite element software iv) Analysis of the results obtained by simulation and validation using results present in the literature. The Altair Flux is a simulation software through the FEM. The software is a reference in the industry and proves to be a high-performance tool in the analysis of electromagnetic problems while providing an easy-to-use environment, thus facilitating the design stages as optimization, data manipulation and visualization of results. In addition to solving electromagnetic simulations, it has an interface with Python programming language that allows automating simulation tests to calculate parameters depending on variation of frequency, variation in conductor excitation, etc. In the context of multiconductor transmission lines, the series impedance matrices and shunt admittance (matrixes [Z] and [Y]) are input data for the models. In the vast majority of the works found in the literature, the shunt conductances of the system are neglected. Therefore, the calculation of the shunt admittance matrix is determined only through the mutual capacitances between the conductors. The capacitance matrix can be calculated in two ways, one procedure determines the terms from the energy stored in the electric field, a second procedure is obtained from the induction of charges in the conductive region calculated based on the electrostatic solution obtained from the FEM. The first approach requires solving a system to determine the mutual capacitances between conductors and then adding the terms to obtain the matrix used in the model, while in the second approach the terms of the model matrix are obtained directly from the induced charges without additional computational effort. In the literature, several similar methods were found for calculating the series impedance matrix. The vast majority of articles studied calculate the matrix based on the concept of power or energy. In other words, the energy stored in the magnetic field and the power dissipated in the conductors is used to calculate the impedances. This procedure is carried out in two steps, initially individual conductors are excited to determine their own series impedance, and then pairs of conductors are excited to determine the mutual series impedances. The concept of mutual resistance between conductors arises from the resistance of the return path for currents. It is also worth pointing out that the series

impedance matrix varies as a function of frequency due to the skin effect of the conductors, which can be saved in a look up table to be easily implemented in conjunction with the model in the frequency domain.

Preliminary results: The procedure presented for calculating the transmission line model matrices was validated using results present in the literature. For all procedures performed, a Python routine was developed to perform the finite element simulations. To validate the calculation of the Capacitance Matrix, a problem obtained from the article “Calculating the Capacitance and Inductance of Multiconductor Transmission Lines” by Sarhan M. Musa and Matthew N.O. Sadiku was used. The article presents the modelling of capacitances and inductances of transmission lines in Integrated Circuits with up to four conductors in a medium with dielectric multilayers. The problem with two conductors and three dielectric layers was chosen. In addition to this work providing numerical results for the problem, it also references an analytical solution for the problem, thus the reliability of the methodology adopted is increased. The results obtained were reasonable. The relative mean error between the values obtained through the Altair Flux software and the numerical solution of the studied paper was less than 1%, as were the relative mean error in relation to the analytical solution. To validate the calculation of the series impedance matrix, results obtained from Yanan Yin's doctoral thesis at Shanghai Jiao Tong University were used. The thesis presents two different methodologies for calculating series impedance, one of which is based on the same concept used to relate impedance to power. The solutions presented in the thesis, unlike other results found in the literature, address different frequency values that vary between 6 Hz and 6 kHz, this way the variation of parameters as a function of frequency can be observed. It is worth mentioning that the thesis consists of the analysis of a coaxial cable with only two conductors and also presents an analytical solution. As with capacitance, the results obtained were identical to the values obtained in the thesis studied for the entire frequency range.

Preliminary conclusions: The methodology used to calculate cable parameters is a well-established method in the literature and is present in several papers studied. Furthermore, the procedure was validated using two existing numerical solutions and the same results were reproduced. Despite the validation of the method, some questions still arise that must be analysed. The method used, despite the FEM being able to model the skin effect on the conductors, neglects the proximity effect between conductors. For overhead transmission lines, the distance between conductors is large enough, in addition with low operating frequency, to neglect the proximity effect. In the case of underground and submarine transmission lines, the cables are more compact and the distance between the conductors is smaller, which makes it necessary to evaluate the influence of the proximity effect in the calculation of the parameters. A second observation for future studies comes from the modelling of the external environment, which influences the calculation of the parameters. As in the case of underground transmission lines, there is a return of current through the earth. There are several methods of modelling this phenomenon, being able to model the external domain through its electromagnetic properties using the FEM, which can excessively increase the simulation domain, or through analytical

methods or other tools such as the image method to correct the influence of the heterogeneous medium. The doctoral thesis used to validate the calculation of the series impedance matrix also presents a solution considering current return through the earth.

Giovani Giulio Tristão Thibes Vieira
Escola Politécnica - University of São Paulo

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Flexible Solutions to increase the hosting capacity of distributed energy resources

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Abstract: The proposed research aims to assess low-cost solutions that enable the system to operate with greater flexibility, in order to increase the hosting capacity of new installations of DER-BTM without deteriorating the quality of power delivered to consumers and prosumers. The rapidly growing number of Distributed Energy Resources Behind The Meter (DER-BTM), especially photovoltaic generation, increases the challenges in operating the grid. These challenges are related to voltage profile degradation, stability margin reduction, feeder overloading, reverse power flow, and decreased performance of the system protection. Different scenarios will be evaluated by the proposed research. Firstly, the hosting capacity of DER-BTM will be evaluated, considering that the distribution utilities have limited control over the number of new installations, their location and their operation. In addition, other scenarios that correspond to solutions with higher controllability levels will also be assessed, considering their maturity levels, and costs of CAPEX and OPEX to be implemented, as presented by the current

literature. This project aims to propose a methodology for power distribution planning that considers the hosting capacity of distributed resources. Thus, the planning engineer will be able to evaluate the impact of different actions over the grid for mitigating distribution feeders congestion, improving voltage profile, contributing to system stability, and considering budget restrictions, over different scenarios for controlling DER-BTM. The project will also consider Distributed Energy Resources Strategically Allocated (DER-SA) as an action that could be performed by distribution utilities to improve the technical performance of the grid. These resources, that could be controlled locally or in a centralized manner, include technologies such as photovoltaic, wind generator, biogas turbines, fuel cells, microturbines, energy storage systems, and load management.

Thus, a complementary objective of the project will be the development of a technical-economic methodology to optimally allocate DER-SA to increase the technical performance of the grid, including its hosting capacity for DER-BTM, considering different costs of the generation and control technologies. The proposed methodologies will be designed considering different MV and LV power distribution grid topologies, which are commonly applied in Brazil or France.

Keywords: Distributed Energy Resources, Hosting Capacity, Optimized Dispach, Enhanced performance of distribution grid topologies.

Introduction and Objectives: Distributed generation (DG) generally refers to the production of electricity by small-scale power generators connected to the distribution system, or on the customer side behind-the-meter (BTM). DG is typically classified into different ratings based on their size and capacity. The four main classical categories of distributed generation are:

• Micro-distributed generation: systems with a capacity of 1 W to 5 kW;

• Small distributed generation: systems with a capacity of 5 kW to 5 MW;

• Medium distributed generation: systems with a capacity of 5 MW to 50

• MW;

• Large distributed generation: systems with a capacity of 50 MW to 300

• MW.

The capacity ratings for distributed generation systems may vary across different regions and countries, but these categories provide a useful framework for understanding the different sizes of distributed generation systems. In Brazil, distributed generation is divided into two categories: microgeneration and minigeneration. Microgeneration is defined as a power plant with installed capacity up to 75 kW, while mini-generation is defined as a power plant with a capacity above 75kW and less than or equal to 3 MW (which may be up to 5 MW in specific situations, in accordance with the regulations). Distributed energy generation has been growing worldwide and, more recently, in Brazil, with an increase of over 17 GW in installed capacity in the last 4 years. Projections indicate that Brazil will have more than 37 GW by 2032. The percentage of each source varied depending on the year, however, in the last years, the increment of photovoltaic has been the predominant technology in the Brazilian DG expansion.

This project aims to develop a methodology for assessing the impact of distributed energy resources on power distribution grids and to evaluate actions made by planning engineers to increase the hosting capacity of renewable energy in distribution systems. The specific objectives are: • To develop detailed computational models for battery energy storage systems, photovoltaic generation, fuel cells, small hydropower plants, biofuel generation, and electric vehicles; • To apply optimization techniques for allocating DER-SA considering specific characteristics of each resource, such as local or centralized control, along with simplified technical-economic analysis that considers the implementation and operation costs of these resources;

• To assess and quantify the benefits from the adoption of an advanced distribution management system for distribution grids, considering different approach towards control alternatives and technology particularities, such as inverter types and configurations, to increase the hosting capacity of DER-BTM;

• To develop a visualization platform, dashboards and reports to present developed scenarios and the impact over MV power distribution grids.

Methodology: The execution methodology is divided into four main parts:

• assessment of distributed energy resources (DERs) in the Brazilian context;

• modelling of DERs;

• static and transient simulations of MV power distribution feeders with DERs behind the meter

(DER BTM); and

• method for strategic allocation of DERs (DER-SA) to increase the hosting capacity of MV power distribution feeders.

Due to the limitation of words, only the first two parts will be detailed.
Assessing Potential Distributed Energy Resources in Brazil
Initially, a review of the state-of-the-art of distributed energy resources will be carried out, taking into account their technological maturity and technical-economic applicability. As aforementioned, photovoltaic generation is the main DER drive in Brazil.

Nevertheless, biofuel is another potential driver for clean DERs [8]. It is noteworthy that most urban cities in Brazil have natural gas distribution infrastructure [9], making it feasible to consider the assessment of natural gas turbines as an option for DER-SA.

Next, the applications of these resources will be evaluated in the regional and economic context of Brazil, seeking to identify the promising opportunities. Once the promising opportunities are identified, a suitable set of resources will be selected. This selection will take into account the technical-economic feasibility, resource availability and CAPEX and OPEX costs.

DER modelling

For the most promising distributed resources, computational simulation models will be

developed for both steady-state and transient simulation. These models will be based on state-of-the-art literature and will incorporate the operational characteristics of commercially available technologies, including ancillary services. The modelling of energy storage, renewable energy, biofuel-based and fuel cell-based power generation is a crucial step in the project. To do so, load and generation curves in distribution systems will be considered, as well as steady-state and transient models. Having the steady-state and transient models developed, a set of generation and demand curves will be created for current and future projections using a public database. These curves will be used to set up scenarios to analyse the potential contribution of each DER to the grid.

Preliminary results: The expected results to be obtained in the proposed project are of interest to power distribution utilities, consumers and prosumers, as well as, of the interest to regulatory agencies and institutions responsible for energetic planning. It is noteworthy that increasing the hosting capacity of renewable energy benefits society as a whole by reducing greenhouse gas emissions. Specifically, the following expected results are listed:
• Mapping of the technological frontier of distributed energy resources in the Brazilian context;
• Methodology for technical and economic analysis for installation and operation of distributed energy resources considering uncertainties;
• Indices to evaluate the performance of distribution grids with distributed generation; • Methodology for optimally allocating DER-SA to improve operation and hosting capacity of distribution grids;
• Visualization platform for the operation and performance of distribution grids; • Formation of highly qualified human resources (post-doctorate; doctorate and master researchers and undergraduate students).

Preliminary conclusions: In this proposal, we presented project 12 from the Power Systems Innovation Hub (InnovaPower) program. In this project's initial phase, we have critically reviewed DER components and standards for integrating these components in the distribution grid. It is impossible to draw any conclusions due to the project phase.

Guilherme Broslavschi Pereira da Silva
Universidade de São Paulo

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Analyse of the impact of distributed generation capacity for voltage and reactive support in distribution system

Authors' Names & Affiliation Institutions of all authors (in order for publication): Guilherme Broslavschi & Universidade de São Paulo.

Abstract: Distributed energy resources (DER) within the scope of distributed generation (DG) connected to the medium voltage distribution network impact voltage levels, which can seriously affect consumers. The increasing integration of renewable energy sources (RES) increases the level of penetration in distribution networks and has a significant impact on the voltage stability of distribution networks, which raises concerns about meeting regulatory requirements such as, for example, the Módulo 8 of the Prodist on power supply quality that determines adequate, precarious and critical voltage levels, and the IEEE Std. 1547 standard that deals with the interconnection and interoperability of DERs with the electric power systems (EPS).

Keywords: Distributed energy resources, distribution network, energy storage, renewable energy sources, voltage stability.

Introduction and Objectives: For the aspects of sustainable energy development, which seeks to improve the level of reliability of the distribution network and solve electric energy supply problems at the most remote points in the power line, DG, such as RES, energy solar photovoltaic, wind and biomass, are growing and receiving more and more attention. DER and

Energy Storage Systems (ESS) that are connected to the grid can change the distribution of power flow, and this trend affects the steady-state voltage distribution of the electric power system. However, if the DG and ESS are allocated rationally, they will play a fundamental role in voltage support in distribution network. On the other hand, the indiscriminate use of DGs without restrictions connected to the electric power grid can cause a phenomenon known as overvoltage.

Methodology: We must first analyse DERs by the characteristics of the reactive power generated by different types of DG or ESS technologies, to support reactive power in electric distribution networks. Next, the concept is proposed that is based on the power transfer margin in the power-voltage curve considering the non-negligible resistance of the distribution network, precisely to quantify and evaluate the voltage stability along the power line when we integrate the DERs with the defined reactive power types. The impact of reactive power losses from distribution lines and transformers on the feeder voltage must also be taken into account.

Preliminary results: Preliminary results show that, according to the various parameters of the

feeder, load capacity and load and DER allocation, the maximum allowable capacity such as the DG peak capacity can be estimated using calculation software of power flow. In which, an analysis of voltage and reactive power levels is carried out to control the capacity of the DER, avoiding overvoltage's and reverse power flow or improving voltage stability in the EPS.

Preliminary conclusions: We conclude that research on the maximum allowable capacity of DERs is necessary, as they can be used to guide and regulate the rational use of this type of intermittent energy, which are RES and ESS, to benefit the functioning of EPS.

Guilherme Fidelis Peixer
Federal University of Santa Catarina

Abstract Title: Performance Assessment of Commercial and Innovative Technologies for Hydrogen Liquefaction

Authors' Names & Affiliation Institutions of all authors (in order for publication): Guilherme Fidelis Peixer (Universidade Federal de Santa Catarina); Jhonatta Bordignon Casagrande (Universidade Federal de Santa Catarina); Yogan Felipe Sganzerla (Universidade Federal de Santa Catarina); Jaime Lozano Cadena (Universidade Federal de Santa Catarina), Jader Riso Barbosa Jr. (Universidade Federal de Santa Catarina)

Abstract: In recent years, hydrogen technologies have attracted growing attention and interest due to their potential to play a crucial role in reducing carbon emissions across various sectors. Nonetheless, fully realizing this potential remains a significant challenge, as technical and economic barriers continue to hinder the widespread adoption of these technologies. Among the major obstacles, storage, and transportation present formidable challenges. Currently, there is a diverse range of alternatives being explored to address these issues, and hydrogen liquefaction has emerged as a particularly promising solution, despite its current high cost and energy-intensive nature. In the pursuit of this goal, a comprehensive assessment of existing technologies has been conducted, encompassing both well-established methods and emerging options for hydrogen liquefaction. Within the domain of well-established technologies, several strategies have been identified as the most promising avenues for enhancing efficiency and reducing costs. These strategies include optimizing various components, integrating hydrogen liquefaction processes with renewable energy sources, implementing innovative cooling techniques, and scaling up traditional energy processes. Meanwhile, among the emerging technologies, caloric systems are still in the early stages of development, with magnetocaloric systems showing the most significant potential for advancement.

Keywords: Liquid Hydrogen, Storage and Transportation, Hydrogen Liquefaction, Caloric Cooling, Magnetic Refrigeration.

Introduction and Objectives: Hydrogen systems are gaining increasing significance in the effort to reduce carbon emissions across multiple sectors. Hydrogen holds the potential to be produced from various primary energy sources and converted into secondary energy forms such as electricity and heat, finding diverse applications, spanning from urban mobility, energy storage, and transportation, as well as industries like chemical, oil, gas, mining, and steel. Currently, global hydrogen production stands at approximately 75 million tonnes per year, while the projected demand for 2050 is estimated to be 621 million tonnes per year. Achieving this ambitious target necessitates addressing several challenges to ensure the anticipated economic, social, and environmental impacts become integral to our energy landscape. The hydrogen value chain can be segmented into four key stages: primary resources, production, storage and transportation, and utilization. At each of them, various alternatives can be employed, resulting in a multitude of pathways from start to finish. However, technical and economic challenges persist within each stage of the value chain, obstructing the efficient application of hydrogen technologies. For example, hydrogen boasts an impressive gravimetric energy density, but its volumetric energy density is notably low, which poses a primary hurdle in the value chain, particularly concerning the development of technologies for effective storage and transport. A range of technologies have been developed over the years to establish a method that is both technically and economically efficient, safe, and scalable to meet global demands. Hydrogen storage technologies are typically categorized into physical and material-based methods. Physical-based methods encompass liquefaction, compression, or a combination of both, whereas material-based methods utilize other substances to bind or react with hydrogen. Although numerous studies advocate for different methods, the suitability of each option largely hinges on the specific technical and economic considerations and the characteristics of the value chain in which it will be employed. Liquefaction proves especially advantageous when high-purity hydrogen is required, as well as in applications demanding high gravimetric energy densities, such as in marine and aviation. Nevertheless, several challenges continue to impede the widespread adoption of hydrogen liquefaction as a viable solution. The primary obstacle is the extremely low liquefaction temperature of -253ºC at atmospheric pressure, which makes liquefaction an energy-intensive process. Furthermore, issues related to scale and safety present additional barriers to the large-scale deployment of current technologies. In light of these challenges, this work aims to conduct a technology assessment of hydrogen liquefaction systems and explore emerging options to uncover innovative solutions for the hydrogen liquefaction process.

Methodology: Hydrogen's journey into liquefied form traces back to 1898 when Sir James Dewar first accomplished this feat. Since then, numerous technologies and system configurations have undergone thorough assessment. Particularly noteworthy among these are the Linde, Claude, and Brayton cycles, regarded as conventional approaches in this discussion. In the past few decades, more than 50 hydrogen liquefaction facilities have been established across Europe, North America, and Asia, although a significant number of them have since fallen into disuse.

Presently, the global hydrogen liquefaction capacity stands at 350 tonnes per day, with the most substantial liquefier boasting a capacity of 32 tonnes per day. Despite considerable advancements in recent years, the performance of hydrogen liquefaction systems continues to require enhancements, both in technical and economic aspects. These improvements are essential to firmly establish the technology as a viable and efficient solution for hydrogen storage and transportation. A critical challenge on this journey is the notably low efficiency of the equipment and processes involved, which stands as a significant impediment to the realization of a robust hydrogen economy. This work seeks to carry out an analysis of the technologies currently employed for hydrogen liquefaction, highlighting their main application field and the challenges and bottlenecks they face for the large-scale adoption of liquid hydrogen as a thermo-economic suitable option as a carrier. The physical principles involved in the conventional systems are evaluated and the advantages and disadvantages of each one are highlighted. As the current scenario is mapped, a screening of innovative alternative technology is carried out, taking into account thermodynamic efficiency, technological maturity, and large-scale adoption perspectives. Among the technologies investigated, there were considered gaseous cycles such as Stirling, Pulse-Tube, Gilford McMahon, heat-activated cycles such as absorption systems, and caloric technologies such as electrocaloric, electrocaloric, and magnetocaloric. Among the alternatives, magnetocaloric systems were deemed to be the most promising technology and the one that is receiving the largest investment from industry and academia; hence it was chosen as the focus of the present work.

Preliminary results: Traditional cycles share common characteristics. In the Linde process, hydrogen undergoes compression and cooling through a sequence of heat exchange steps, achieved either with the returning hydrogen stream or through pre-cooling using auxiliary fluids. In the final phase, an expansion device is employed to further cool the hydrogen through the Joule-Thomson effect. The Claude cycle, on the other hand, integrates an expansion engine with Joule-Thomson expansion. Here, hydrogen is compressed and subjected to a series of heat exchange processes, with expansion engines placed strategically between the inlet ports of certain heat exchangers. A portion of the hydrogen flow is directed to these engines, where it is expanded, cooled, and utilized to lower the temperature of the primary hydrogen stream while generating useful work. This cycle can achieve higher energy efficiencies and operate at lower pressures, making the pre-cooled Claude cycle the choice for most hydrogen liquefaction plants. The Brayton cycle, meanwhile, employs auxiliary fluids as refrigerants, enabling lower hydrogen stream pressures and the liquefaction of higher percentages of hydrogen. Advancements in conventional cycle components encompass the use of innovative refrigerant mixtures, high-efficiency compressors, turbines, cascading of cycles, and hybridization with renewable energy systems. Various system architectures have been explored, involving arrangements of pre-cooling loops, compressors, refrigerant mixtures, heat exchangers, and expanders. However, existing literature indicates that altering cycle configurations does not hold significant promise for reducing plant energy consumption. Therefore, the exploration of novel cooling technologies emerges as a potential avenue to achieve this objective. Among these technologies, magnetocaloric cooling stands out as holding substantial potential. This

method offers several advantages, including the absence of harmful fluids, the potential for high levels of efficiency, substantial magnetocaloric effects, and the opportunity to employ superconducting magnets. In terms of prototypes, Kim et al. (2013) developed a two-stage active magnetic regenerator capable of operating between 77 K and 20 K, utilizing four different magnetocaloric material alloys and a superconducting magnet. This setup achieved a minimum temperature of 24 K. Numazawa et al. (2014) proposed a system for liquefying 10 kg/day of liquid hydrogen using a magnetic refrigerator. The liquefaction stage's efficiency was assumed to be 50% of the Carnot efficiency. Feng et al. (2020) introduced a similar configuration, where active magnetic regenerators were employed in cascade stages and crossed by helium streams. The helium streams were used to cool the hydrogen stream from 80 K to 20 K. The authors targeted a liquefaction rate of 300 kg per day, and the maximum second law efficiency reached 76.9% and 67.5% for temperature spans of 5 K and 20 K, respectively.

Preliminary conclusions: Hydrogen systems are poised to play a pivotal role in the worldwide transition toward a more sustainable and resilient energy landscape. However, their anticipated impact is currently impeded by a set of economic and technical challenges. A prominent hurdle in this journey is the storage and transportation of hydrogen, primarily due to its low density, where hydrogen liquefaction emerges as a promising solution. Nevertheless, hydrogen liquefaction remains a costly and energy-intensive process, lacking the capacity required to accommodate the projected surge in hydrogen demand in the coming years. Among the established systems, namely the Claude, Linde, and Brayton cycles, various conceptual frameworks have been developed to align with both technical and economic objectives. Significant potential for improvement lies in the design and optimization of key components, notably heat exchangers, expanders, and compressors. One of the most promising strategies for cost reduction in hydrogen liquefaction plants involves scaling up the systems, although this approach demands careful consideration of the associated investment costs. Another avenue for enhancing system efficiency is the integration of conventional cycles with renewable energy sources, alongside the incorporation of novel cooling techniques such as absorption technology. Crucially, validating proposed designs through the actual construction and operation of conceptual plants outlined in the literature is vital for their practical implementation. Regarding emerging technologies, magnetocaloric cooling stands out among caloric alternatives, demonstrating significant potential. However, for this technology to effectively meet the anticipated global demand for hydrogen liquefaction and reduce operating costs, a shift in focus toward larger liquefaction capacities is imperative in its development.

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Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Optimized RED allocation to increase distributed renewable generation hosting capacity

Authors' Names & Affiliation Institutions of all authors: Orientador: Mauricio B C Salles - Professor Doctor Universidade de São Paulo - Poli - USP Orientando: Leandro Oliveira Martins - Master's Degree student Universidade de São Paulo - Poli – USP.

Abstract: With the increasing number of distributed energy generation, especially photovoltaic generation, challenges in grid operation increase. These challenges are related to the degradation of the voltage profile, reduction of the stability margin, feeder overload, reverse power flow and decreased performance of the system's protection mechanisms. The proposed research aims at low-cost solutions that allow the system to operate with greater flexibility, it also includes evaluating normative references of international standards for the integration of photovoltaic systems into the distribution system, in order to increase the hosting capacity of new DER-BTM installations without deteriorating the quality of energy delivered to consumers. in the initial stages of the project, key national and international standards were evaluated regarding the integration of renewable sources into the distribution system, as well as a comparative analysis of the main requirements and indicators of quality and safety of the system. The development of an economical technical methodology to allocate DER-SA in an optimized way to increase the technical performance of the network, including its hosting capacity for DER-BTM, considering different costs of generation technologies and control.

The proposed methodologies were designed considering different MV and LV topologies, this methodology portrays the five main stages of this project. Furthermore, as this project is in its initial phase, no results or conclusions can be provided.

Keywords: Method for strategic allocation of DERs (DER-SA), Develop a solid base of international references and regulations, standards, Evaluation of distributed energy resources, hosting capacity, photovoltaic generation, grid operation.

Introduction and Objectives: In the coming years, a 37 GW increase in distributed generation capacity is expected, the majority of which will be supplied by photovoltaic generation installed on consumers' rooftops. This increase in behind-the-meter distributed energy resources (DER-BTM) will lead to many challenges in grid operation. For this reason, this work seeks to carry out in-depth and dynamic research on international regulations and standards to understand the integration, security and stability criteria models adopted outside Brazil, in order to create a definition of the relationship control model between customers and Dealers in regions where

the development of norms and standards is more evolved, in addition, the review of these norms is an essential step of this project, this will keep us updated on the integration of these participants of new energy sources (batteries, solar photovoltaic, wind, vehicles electrical and others). These references bring us the state of the art of the process itself and are extremely important for this research work in addition to composing a piece that is in constant dynamic Evolution. The main challenges of the electrical system with distributed generation are related to voltage profile degradation, reduced stability margin, feeder overload, reverse power flow and decreased system protection performance. The proposed research aims to evaluate solutions that allow the system to operate with greater flexibility, in order to increase the accommodation capacity of the new DER-BTM, taking into account what has been said, all the analysis that will be carried out in this project will be from the perspective of the energy distributor DER-SA, always paying attention to the application of best engineering practices and resource planning tasks that aim to optimize the use of the network and mitigate the negative effects that the insertion of distributed sources can cause to the electrical distribution system. This project aims to develop a methodology to evaluate the impact of energy resources distributed in energy distribution networks and evaluate the actions carried out by planning engineers to increase the hosting capacity of distributed energy in distribution systems These are the main objectives of the project:

● Develop a solid base of international references and regulations in order to know the best solution implemented in other countries that can be adopted in Brazil reality, with regard to integration processes, security and control criteria and indicators of power quality.

● Apply optimization techniques for DER-SA allocation considering characteristics of each resource, such as local or centralized control, together with simplified technical-economic analysis that considers the implementation and operating costs of these resources;

● Develop a visualization platform, dashboards and reports to present scenarios and the impact on MV energy distribution networks.

Methodology: The execution methodology is divided into five main parts:

•Evaluation of distributed energy resources (DERs) in the Brazilian and global context so that a review of the state of the art of distributed energy resources will be carried out, taking into account their technological maturity and technical-economic applicability with a focus on DER-AS; ● Develop a solid base of international references and regulations in order to know the best solution already implemented in other countries and that can be adapted to the Brazilian reality, with regard to integration processes, security and control criteria and indicators of power quality; •For the most promising distributed resources, computational simulation models will be developed for both steady-state simulation a focus on DER-AS;

•Method for strategic allocation of DERs (DER-SA) to increase the hosting capacity of MV power distribution feeders. As the DER-SA category refers to resources strategically allocated by the electricity distribution concessionaire, the optimal allocation will take into account which DER are most likely to be installed by consumers (DER-BTM) and which have the potential to help the concessionaire to improve feeder operation;

•Validation by Simulation via Opem DSS (or similar) of the impact of DER-SA on distribution networks using optimization mechanisms to verify loads and network indicators.

Preliminary results: Preliminary Results

Given the initial phase of the project, the results are in the bibliographical review phase, with no significant results worth mentioning yet.

Preliminary conclusions: Preliminary Conclusions

Given the initial phase of the project, the conclusions are in the bibliographic review phase,

with no significant results worth mentioning yet.

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Institute of Energy and Environment - USP

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Abstract Title : Investigation of offshore transmission technologies on the Brazilian coast applied in oil and gas exploration and wind farm integration ("TransBRcoast")

Authors' Names & Affiliation Institutions of all authors (in order for publication) *Renato Monaro (Poli-USP), Maurício Salles (Poli-USP), Luís Felipe Normandia Lourenço (IEE-USP), Rodolfo Varraschim Rocha (UFMT), Liciane Otremba (Poli-USP), Muhammad Zubair (Poli-USP), Bruna Cardozo de Lima (Poli-USP), Isabela Corrêa Hilal (Poli-USP), Vinicius Cerqueira (Poli-USP).

Abstract: This research project aims to evaluate the integration of offshore wind farms and O&G (oil and gas) exploration plants into Brazil's power grid, considering different transmission technologies for the connection of future developments planned to be installed along the Brazilian coast in the following decades. To determine the most adequate transmission technology for each type of development, technical and economic aspects of each alternative will be considered. Protection, control and stability analysis of the transmission technologies based on power converters will be evaluated in the laboratory by performing real-time simulation with power hardware in the loop, using a real multi-level converter with reduced

voltage. A technical-economical tool will be developed to support the definition of new offshore transmission systems based on the distance from shore, seabed depth, and total power of the wind farms and O&G plants. Furthermore, new protection and control techniques may be proposed to satisfy the offshore transmission system's requirements if necessary. The project is divided into six activities: a survey of offshore transmission systems to determine the technologies applicable in Brazil's case; development of a technical-economical tool to guide future offshore transmission projects; mathematical modeling of the offshore transmission technologies to be used in stability, control and protection studies; computational simulation using the models defined in the previous activity, different transmission technologies will be simulated based on future real cases to be implemented on the Brazilian coast; improvement and proposition of control and protection techniques for the offshore transmission systems, considering the cases simulated in the previous activity; and simulations using a real-time platform with real equipment in a power-hardware in the loop configuration. Within this context, this project aims to produce a series of methodologies so that the evaluation can be systematically conducted, providing a technical and scientific basis for expanding transmission systems to the sea. Therefore, it corroborates with the increase of wind energy in the energy transition and the decarbonization of O&G exploration in Brazil and worldwide.

Keywords: Power Transmission, Offshore Wind Farms, Offshore Transmission, Power From Shore, Power to Shore.

Introduction and Objectives: Climate change is a pressing global matter that demands urgent action. The pressure on governments worldwide to set ambitious targets for adopting sustainable energy sources is growing as the general public becomes aware of the negative environmental impacts of traditional power sources. An essential action toward a solution to the climate crisis is the adoption of renewable energy sources to reduce greenhouse gas (GHG) emissions in the energy sector.

Following this trend, wind power generation rose to 1600 TWh in 2020. The economic feasibility of wind power is tied to the geographical locations where its primary resource is favorable for electricity generation, which does not translate directly into proximity to the load centers or the existing transmission lines. Additionally, concerns over visual and noise pollution allied with steadier and higher wind speeds are pushing for offshore wind power exploration, which in the Brazilian context, will require a new dedicated power transmission infrastructure.

Even with the increased emphasis on green energy sources, Oil and Gas (O&G) are still expected to play a crucial role during the clean energy transition. However, O&G production processes are energy intensive. To mitigate this, new policies such as carbon taxation were implemented, and it's crucial to maintain O&G competitiveness by producing them with as low GHG emissions as possible. One way to reduce the carbon footprint of O&G production processes is by integrating production platforms with onshore renewable energy sources. This connection with the onshore grid is referred to as Power From Shore (PFS). In parallel with the power from shore scenario, the expansion of offshore electrical networks has also been driven

by the development of offshore wind farms. Although the onshore wind farm projects correspond to 93% of the global wind power in operating projects, offshore wind turbine applications are distinguished by their vast energetic potential due to superior wind speed and stability compared to an equivalent project onshore. The increase in power capacity of recent wind turbines is opening up new frontiers in the form of large offshore wind farms. The concept of generating power offshore and transferring it to the onshore grid is referred to as Power To Shore (P2S). This project's main objective is to study offshore electrical transmission systems on the Brazilian coast for both P2S and PFS applications. The transmission technologies High Voltage Direct Current (HVDC), High Voltage Alternating Current (HVAC), and Low-Frequency Alternating Current (LFAC) will be investigated. The specific objectives are listed as follows:

Evaluation of applicable offshore transmission technologies and topologies to the Brazilian coast; Development of a simplified technical and economic analysis tool for the studied transmission technologies; Study of stability, control, and protection of different types of offshore transmission systems.

Methodology: Survey on offshore transmission Technologies:

The technical and operational characteristics of HVAC, HVDC and LFAC systems will be investigated. The survey will include research in databases, to determine the technologies to be used and the characteristics of the offshore wind farms and O&G. Examples of real developments worldwide will also be considered.

Development of a technical-economical tool

A systematic technical and economical procedure will be developed to assist in identifying the key features of feasible transmission systems based on the topologies defined on the literature survey. The procedure will help to determine if the considered transmission systems meet the necessary technical requirements. This analysis will be based on steady-state power flow models. If the system meets the requirements, the tool will also provide an estimated cost of the transmission infrastructure. Modeling of offshore transmission components

The transient analysis of the three transmission technologies (HVAC, HVDC and LFAC) for the PFS and P2S applications will be based on computational simulations, which require the mathematical models of the components. Therefore, during this part of the project, these models will be developed, if needed, or adapted from other applications. The proposed models will be developed and tested using Matlab/Simulink, which will also be used for the computational and PHIL simulations. The equivalent model of the wind farm and O&G platforms will also be developed to perform simulations focused on the transmission line. These models will combine the dynamic response of its equipment; for example, a wind farm will be modeled as an equivalent wind generator with power proportional to the number of turbines within the farm. A similar procedure will be used for the O&G plants.

Computational Simulations

Steady-state and transient studies of the investigated transmission systems will be performed. Steady-state analysis will provide relevant information for sizing the transmission system. The

transient regime analysis will be relevant to evaluate the control, protection and stability techniques of the system as a whole. Test cases, based on the real future developments will be simulated. These analyses will be carried out considering the individual and mutual contributions of wind farms and O&G plants, as these may share the transmission system for the coast.

Power-Hardware in the Loop Simulation

The Power-Hardware in the Loop (PHIL) simulations will focus on the transmission system, specifically on the converter stations of the LFAC and HVDC systems. Simulations of each presented topology will be conducted to evaluate the behavior of electrical networks under normal and abnormal conditions. These simulations will be performed using a OPAL-RT PHIL platform and real converters and generators.

Preliminary results: This project has started recently; hence partial results are yet to be obtained. The expected research results are particularly relevant to the energy industry and its stakeholders, including investors. These findings can have an impact on investment decisions, making them more informed and beneficial. In The main expected results are:

Mapping of the technological frontier of submarine transmission systems with potential for implementation on the Brazilian coast;

A computational tool for simplified technical-economic analysis for subsea transmission technologies; Verification of the applicability of controllers of different transmission technologies applied to offshore systems;

A survey of the limitations of the technologies studied in relation to stability, control strategies and the needs of the protection system;

Control and protection techniques adapted to the offshore transmission system; A database with the mathematical models of the offshore transmission components; A library with the control and protection algorithms proposed;

Training of highly qualified human resources.

Preliminary conclusions: In this abstract we introduce project #08 within the InnovaPower program that is ongoing for 3 months at the moment of the submission. This project aims at studying transmission system alternatives for the new offshore transmission infrastructure that will be required for offshore wind exploration and to eventually interconnect O&G production units to the onshore grid. The methodology of the project was described alongside the expected results.

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Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Automated Circuit Construction for Resonance Analysis in Distributed Energy Resource Integration

Authors' Names & Affiliation Institutions of all authors (in order for publication):
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Affiliation: Universidade de São Paulo (USP)
Maurício Barbosa de Camargo Salles
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Abstract: The increasing integration of Distributed Energy Resources (DERs) with power electronic interfaces has a still poorly understood impact on the power quality of grids. The power electronic converters in DERs may exhibit negative resistance at certain frequencies, which can affect circuit damping and cause resonances in the system. Currently, there are no effective methods for analyzing and mitigating these resonances. Developing simplified methods for assessing and identifying critical resonance scenarios in low and mediumvoltage systems requires time-consuming grid simulation, with numerous configurations. In this context, we aim to develop a computational tool to automatize the construction of the simulated circuits in software.

Keywords: Automation, Distributed Energy Resources, Resonance, MATLAB.

Introduction and Objectives: Electric power distribution systems are undergoing a significant transformation, shifting from passive and low-level automation to active and highly automated operation. This advancement is driven by the introduction of Distributed Energy Resources (DERs), such as photovoltaic and wind generators, which are connected to the electrical grid through power electronic converters [1, 2]. Additionally, the deployment of automatically operated capacitor banks is becoming more common in both medium voltage (MV) and low voltage (LV) networks to improve power quality and system efficiency [4]. However, the increasing presence of DERs and capacitor banks can potentially trigger circuit resonances. Power electronic converters used in DERs, such as voltage source converters, exhibit negative resistance characteristics at certain frequencies. When this negative resistance aligns with the circuit's resonance frequency, weakly damped or even unstable resonances may occur, leading to damage to electrical equipment and potential financial losses for distribution utilities and customers [3]. The evolution of power distribution systems with the growing adoption of DERs and automatically operated capacitor banks represents a significant advancement in the pursuit of greater efficiency and reliability. Nevertheless, the coexistence of these elements also

presents challenges, particularly concerning circuit resonances. Understanding these interactions is crucial to ensuring the stability and safety of the electrical system. Research and development of new methods to systematically assess the risk of resonances based on grid characteristics, without requiring a large amount of time, resources, and specialized knowledge, is essential. Developing suitable theoretical models is crucial for this approach, and computer simulations are a necessary part of the process. Building grids with various topologies is time-consuming and inefficient, so automating these procedures can significantly accelerate development. This project aims to facilitate the simulation of different configurations and topologies of distribution systems with high DER penetration in the Simulink software by automating the grid construction process.

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[2] G. Mauri, F. Pilo, J. Taylor, G. Bruno, E. Kampf, F. Silvestro, C. Pecas Lopez, B. Bak-Jensen, J. R. Pillai, and H. Sprongl. "Control and Automation Systems for Electricity Distribution Networks (EDN) of the future", CIGRE/CIRED Joint Working Group, 2017.
[3] Y. Song and F. Blaabjerg, "Analysis of the Behavior of Undamped and Unstable High Frequency Resonance in a DFIG System," IEEE Transactions on Power Electronics, vol. 32, no. 6, pp. 4370–4394, 2017 [4] V. L. Holsomback, "Capacitor monitoring systems and methods of metering and monitoring capacitor bank." U.S. Patent No. 8,547,109, 2013.

Methodology: The methodology of this project encompasses the analysis and characterization of the functionalities required to address the proposed problem. The tool to be developed should be able to process grid information taken from the Geographic Database of the Distribution Company (Base de Dados Geográfica da Distribuidora, BDGD) provided by the National Electric Energy Agency (Agência Nacional de Energia Elétrica, ANEEL) and automatically construct them in Simulink. The resource will be based on MATLAB code, and the interface between the code and the data will be implemented in Python.

Preliminary results: MATLAB includes a library of functions that enables direct code

interaction with Simulink, allowing for the automatic construction of networks based on code-defined parameters. To explore and understand these functionalities, a small draft code was developed.

Preliminary conclusions: The project is still in its early stages, so no Preliminaryy conclusions can be drawn.

SHORT ORAL SESSION C

11h30 - Short Oral Session C

0811 – EnvSG9 (TV1)

Chairs: Suani T. Coelho – Edmilson M dos Santos

Alberto Torres Riera Junior
University of São Paulo

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP) and sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by Petronas, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: A Machine Learning Force Field for Boric Acid and Water

Authors' Names & Affiliation Institutions of all authors (in order for publication): Institute of Physics, University of São Paulo.

Abstract: The management of produced water (PW) is a critical process within the Oil and gas (O&G) exploration and production industry. PW constitutes a substantial volume of waste generated at production plants, primarily those situated on offshore platforms. In recent times, PW has garnered global attention due to its immense potential to alleviate freshwater scarcity and its potential for reuse in irrigation systems. However, PW is a complex mixture of organic and inorganic components, including a significant presence of toxic elements, which poses challenges for its safe and efficient reuse. In this work, we build a Machine Learning force field to perform molecular dynamics simulations with ab-initio accuracy at much lower computational cost.

Keywords: Produced Water; Boron; Machine Learning.

Introduction and Objectives: The management of produced water (PW) is a critical process within the Oil and gas (O&G) exploration and production industry. PW constitutes a substantial volume of waste generated at production plants, primarily those situated on offshore platforms. In recent times, PW has garnered global attention due to its immense potential to alleviate freshwater scarcity and its potential for reuse in irrigation systems. However, PW is a complex mixture of organic and inorganic components, including a significant presence of toxic elements, which poses challenges for its safe and efficient reuse. Notably, PW exhibits a high concentration of Boron (B) [PSEP 92, 509-514 (2014)]. Boron is an essential element for animals, plants, and humans. However, prolonged exposure to high levels of B in water can be

detrimental to plant growth and pose significant health risks for humans and animals, affecting the functioning of some organs. According to the World Health Organization (WHO), the acceptable amount of B in drinking water is 2.4 mg/L and 0.5 mg/L for irrigation water. To meet WHO requirements, innovative and efficient technologies for B removal from PW are necessary. Several water treatment technologies are available for B removal. Among these technologies, membrane-based approaches are considered the most promising and effective. However, when it comes to removing B and its compounds, membranes face an additional challenge. Boron occurs naturally in various forms, including boric acid and borate salts. Studies have demonstrated that the rate of B removal is directly influenced by pH levels. Additionally, Capacitive Deionization by Membrane (CDI) has shown considerable potential for water recovery and efficient B removal. From the perspective of materials science, computational methodologies can provide insights into processes occurring at the atomic scale. They are also valuable due to their ability to explore a wide range of systems. One of the key innovations is the integration of Materials Informatics, multiscale molecular simulations, machine learning, and topological optimization to expedite screening and selection, subsequently allowing for the design of systems that optimize the selectivity of B within nanostructured materials.
In this work we have built a Machine Learning force field (MLFF) using data obtained from accurate first principles calculations of boric acid solvated in water. This MLFF will allow us to perform molecular dynamics simulations with ab initio accuracy at a much lower computational cost.

Methodology: Initially, phase (geometric configuration) sampling was conducted using empirical potentials obtained from the literature: Risplendi's potential for boric acid [J. Phys. Chem. C 124, 1438–1445 (2020)], and q TIP4P-F potential for water [J. Chem. Phys. 131, 024501 (2009)]. Molecular dynamics (MD) simulations were performed using the LAMMPS code at various temperatures, pressures, and concentrations, from which several thousand uncorrelated geometries were extracted.
First-principle single-point calculations were conducted using density functional theory (DFT), implemented in the SIESTA code (https://departments.icmab.es/leem/siesta). These calculations utilized a localized double polarized basis set, an exchange-correlation functional that includes van der Waals interactions (optB88-vdW [J. Phys.: Condens. Matter 22, 022201 (2010)]), and a tight integration mesh. The purpose of these calculations was to obtain precise energies, forces, and the stress tensor (e.g., pressures) for each configuration obtained in the phase sampling.
The MLFF was generated by training neural networks (NN) using a modified version of the DEEP-MD code (https://github.com/deepmodeling/deepmd-kit), where a term was added to the loss function to (softly) impose conservation of momentum, improving correctness and, at the same time, adding a regularization term to the training process. The NNs were trained until the energies, forces, and pressures (via stress tensors) were converged within the desired accuracy.

Preliminary results: A machine learning force field to describe a solution of boric acid in

water was generated. This MLFF correctly describes the interaction of boric acid and water molecules. The errors of the energies, forces, and the virial term given by the MLFF obtained in this work relative to the density functional calculations are within chemical accuracy: ~1 meV/atom, ~0.04 meV/Å, and ~0.1 eV, respectively.

Preliminary conclusions: The machine learning force field created in this work correctly describes the interactions of the atoms in boric acid, water, and between both, generating forces and energies with ab initio accuracy, allowing us to perform molecular dynamics simulations with high accuracy (at the level of theory described above) at a fraction of the computational cost.

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Abstract Title: Addressing Cumulative Impact Assessment into the planning and development of offshore wind farms on the Brazilian coast

Authors' Names & Affiliation Institutions of all authors (in order for publication):

Ana Paula Alves Dibo (Escola Politécnica, University of São Paulo), Carla Grigoletto Duarte (Universidade Federal de São Paulo), Alexander Turra (Instituto Oceanográfico, University of São Paulo), Luis Enrique Sánchez (Escola Politécnica, University of São Paulo).

Abstract: Offshore wind energy has been expanding worldwide significantly due to the energy transition towards a low-carbon economy. Brazil can play an important role in expanding its energy matrix based on renewable energy with offshore wind energy. Despite wind energy being a renewable and clean source, several environmental impacts have been linked to the activity in different countries. For issuance of an environmental license for offshore wind energy projects, an Environmental and Social Impact Assessment (ESIA) should be submitted to Ibama for analysis. It is also important to develop environmental and social assessments at strategic levels to support the planning of expanding offshore wind energy, especially considering the effects of multiple activities in marine and coastal spaces. Cumulative impact assessment (CIA), an internationally recognized and recommended practice, is one of the

approaches to impact assessment that can be applied at both strategic and project levels, especially considering that cumulative impacts of offshore wind farms are an increasing concern when discussing marine planning and development, in association with existing and planned activities. Despite the requirements, CIA practice in Brazil is underdeveloped. Based on the relevant role that the CIA can play in the decision-making process of the offshore wind energy sector, this research has the aim to provide guidelines for addressing the CIA in the planning and development of offshore wind farms on the Brazilian coast. For that purpose, it will be conducting the following steps: (1) survey of environmental regulation of offshore energy development to Cumulative Impact Assessment; (2) state of-the-art of Cumulative Impact Assessment of offshore wind energy; (3) development of practical guidance for Cumulative Impact Assessment of offshore wind energy; and (4) discussion of potential cumulative impacts on the Brazilian coast. This research is part of the project EnvSoOff developed, under the coordination of Prof. Luis E. Sánchez, as one component of the research agreement between USP and TotalEnergies, in the InnovaPower Program, coordinated by the Research Centre for Greenhouse Gas Innovation (RCGI) of POLI-USP.

Keywords: cumulative impact; impact assessment; marine spatial planning; offshore wind energy.

Introduction and Objectives: Offshore wind energy has been expanding worldwide significantly, driven by the energy transition towards a low-carbon economy, and Brazil has a great opportunity to expand its energy matrix based on renewable energy with offshore wind energy. Although offshore wind energy is a renewable and clean source, several environmental impacts have been linked to the activity in different countries. Like any activity that causes significant environmental degradation, an Environmental and Social Impact Assessment (ESIA) is required as part of the environmental licensing process; whose competent authority is Ibama in Brazil. Moreover, it is necessary to support a holistic marine management and sustainable development goals (Willsteed et al., 2018), considering multiple uses of marine space, such as fishing, tourism and oil and gas activities (EPE, 2020). Approaches to impact assessment in support of environmental licensing decisions in early stages include strategic environmental assessment (SEA) and its links with marine spatial planning, the project ESIA – the latter in support of environmental licensing decisions – and Cumulative Impact Assessment (CIA), which can be applied at both strategic and project level. CIA is an internationally recognized and recommended practice in ESIA of development proposals, which has been a key element of good-practice impact assessment in the countries (IAIA, 2017). It aims at assessing project impacts in combination with the impacts of other developments (from past, present, and future) in specific environmental and social valued components. CIA can support more informed decisions, especially when there is a spatial concentration of undertaking that can cause cumulative impacts (Ma; Becker; Kilgore, 2009; Connelly, 2011; IFC, 2013), and it is also recommended to be integrated within the context of SEA-driven approaches (Harriman; Noble, 2008). Cumulative impacts for offshore wind farms are an increasing concern when discussing marine planning and development, especially those on the flora and fauna, and that

are not identified when assessing only a single wind farm (Köller; Köppel; Peters, 2006). Considering CIA practice as a fundamental need in the Brazilian context (Duarte; Dibo; Sánchez, 2017; Dibo, 2018), the role that CIA can play in the decision-making process on expanding the offshore wind energy sector in Brazil aiming to sustainable development goals and bearing in mind that assessing cumulative impacts on ecosystem is a major challenge both to scientists as well as managers (Raoux et al., 2018), the research has the aim to provide guidelines for addressing Cumulative Impact Assessment in the planning and development of offshore wind farms in the Brazilian coast. This research is part of the project EnvSoOff – Assessment of the environmental and social impact of offshore wind energy (InnovaPower Program / RCGI).

Methodology: The research comprises four steps, as described below.
In Step 1 – Survey of environmental regulation of offshore energy development to CIA, it will be developed a survey of environmental legislation and policy of offshore energy development currently in usage in different countries regarding conducting CIA at both strategic, regional, and project levels, to discuss what are the existing requirements related to cumulative impacts included in legislation and policy of offshore energy development. In addition, available guidance will be reviewed to meet the legislation requirements to incorporate cumulative impacts. The target countries for the review will be selected under the scope of the EnvSoOff project. The research will be conducted by considering the available information on the official websites of each country, reports, academic research, scientific articles, and other sources found. Step 2 – State-of-the-art of Cumulative Impact Assessment of offshore wind energy aims at surveying the current practice of CIA for offshore wind energy in environmental impact assessments, strategic environmental assessments, regional assessments, and other documents of interest, based on a search of governmental databases of the selected countries in Step 1. The review will be based on questions guided by a set of CIA good-practice criteria derived from the literature and based on the criteria applied by, for example, Willsteed et al. (2018). A similar process will be applied in Brazil to select a sample of environmental impact statements available at Ibama's repository of environmental studies. Moreover, special notes will be presented on the potential cumulative impacts of wind energy and other types of development, such as oil and gas projects, in selected valued components, considering the source pathway-receptor model (CEAA, 2018).
Step 3 – Development of practical guidance for Cumulative Impact Assessment of offshore wind energy aims at preparing practical guidance for Cumulative Impact Assessment of offshore wind energy development in the Brazilian context, both to assist the definition of regulatory requirements and decision-making process and to support developers in assessing and managing cumulative impacts. It will also be discussed opportunities to support the CIA for regional marine management and marine spatial planning. For that purpose, it will be considered the findings of the previous steps and an additional literature review will be conducted, aiming to outline the guidelines.

Based on the findings of Step 3, Step 4 – Discussion of potential cumulative impacts on the Brazilian coast, aims to discuss the potential cumulative impacts in a specific location on the Brazilian coast, which will be further selected under the scope of the EnvSoOff project.

Preliminary results: The development of the project advances in the selection of countries under the scope of the EnvSoOff project, to discuss what are the international requirements related to cumulative impacts included in legislation and policy of offshore energy development. The countries selected were: China, the United Kingdom, the United States, Australia and the Netherlands, based on the following criteria: the installed capacity of offshore wind energy, the existence of expansion targets for this type of project in the coming years, and the existence of a consolidated environmental impact assessment system.

Preliminary conclusions: The project is expected to contribute to the integration of Cumulative Impact Assessment in the decision-making process on expanding Brazil's offshore wind energy sector.

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03 - Assessment of the environmental and social impact of offshore wind energy ("EnvSoOff")

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Assessment of the environmental and social impact of offshore wind energy ("EnvSoOff")

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Abstract: This research project aims at developing a framework for the assessment and mitigation of environmental and social impacts of offshore wind farms on the Brazilian coast, grounded on the ecosystem approach and international best practices. For that purpose, we will: (1) survey environmental regulation of offshore energy development in selected countries; (2) collate the state-of the-art of environmental and social impact assessment practices of offshore wind energy; (3) develop a conceptual model for environmental and social impact assessment of offshore wind energy development; (4) prepare a baseline of benthic and pelagic communities, building a georeferenced (GIS) map of biodiversity, in the continental shelf of the study area; and (5) compile information on legislation, public policies, and actual and potential uses of the maritime space develop an integrated analysis of potential conflicts and synergies of offshore wind farms in the context of Marine Spatial Planning (MSP). The ideal

strategy is to predict the sensitivity of marine ecosystems to possible impacts, making it possible to design conservation strategies and protection measures. Some potential impacts on biodiversity and ecosystem services associated with fixed-bottom offshore wind farms are known: changes in seabed habitats and hydrodynamics; habitat creation; changes in trophic webs; barrier effects or displacements; mortality, injuries and behavioural effects associated with vessels and underwater noise; behavioural effects associated with electromagnetic fields from submarine cables; pollution (e.g. dust, light, solid/liquid waste); indirect off-site impacts due to increased economic activity and displaced activities such as fishing; impacts associated with ecosystem services; introduction of invasive alien species. The use of MSP, understood as a public process of analysis and attribution of the spatial and temporal distribution of human activities in marine areas, aiming to achieve ecological, economic, and social objectives, generally specified through a political process, proposes to integrate aspects of the use of space marine environment with biodiversity, in a complex approach that requires a systemic, inter and transdisciplinary perspective. However, in Brazil, the MSP still lacks a legal instrument to support it. In this sense, it is essential to reinforce public policies that allow promoting a systemic vision of the maritime territory, valuing its vocations, protecting its vulnerabilities, and thus developing its potential. This idea is the MSP initiative, which is intended to be developed within the scope of this project, which aims to develop offshore wind energy on the Brazilian coast. Therefore, this project will seek to organize information on marine biodiversity to support decision-making with the perspective of implementing this renewable energy source in marine areas on a sustainable basis.

Keywords: Marine biodiversity; biota sensitivity; ecosystem services; cumulative impacts; Marine Spatial Planning; decision making.

Introduction and Objectives: Offshore wind energy has been expanding worldwide significantly, driven by the energy transition towards a low carbon economy. Technological innovation has been underpinning the construction of large capacity systems and lowering costs.

Approaches to impact assessment in support of decisions on siting, construction, operation and decommissioning of wind energy facilities include Strategic Environmental Assessment (SEA) – and its links with Marine Spatial Planning (MSP), Cumulative Impact Assessment (CIA) and project Environmental and Social Impact Assessment (ESIA), the latter in support of environmental licensing decisions. Offshore wind energy development is at initial stages in Brazil. This represents an opportunity to plan its expansion on sustainable foundations, respecting the carrying capacity of coastal and ocean environments and considering the perspectives of different stakeholders, including local communities. The main objective of this research is the development of a framework for assessing the environmental and social impacts of offshore wind power undertakings in the Brazilian coastal area. The associate objectives are:

- To survey environmental regulation of offshore wind energy in selected countries and equivalent Brazilian regulations;
- To survey the state-of-the-art of environmental and social impact assessment of offshore wind

energy development;
- To prepare an activity-aspect-impact-mitigation causal chain for offshore wind energy development and EIA guidance for the sector;
- To prepare a georeferenced baseline map (GIS) of biodiversity, in the continental shelf of the study area;
- To compile information on legislation, public policies, and actual and potential uses of the maritime space; and
- To develop an integrated analysis of potential conflicts and synergies of offshore wind farms in the context of Marine Spatial Planning.

Methodology: Component 1: Review of environmental legislation of offshore energy in selected countries. The main product is a summary of key regulations relative to environmental impact assessment, marine spatial planning and project environmental management and follow-up, including a summary comparative table and a set of best regulatory practices applicable to the Brazilian context.
Component 2: Selected environmental impact studies and other documents pertaining to projects in the selected countries will be reviewed, alongside an extensive literature review. The key products are: (i) standard lists of activities, environmental aspects and impacts, and corresponding mitigation, with corresponding explanatory notes, and (ii) a review of the extent to which cumulative impacts are addressed. Component 3: This activity will map impact causal chains and produce impact matrices, tables to facilitate screening of other developments to assess cumulative impacts, guidance to determine impact significance and a set of indicators to evaluate outcomes of mitigation. This component will be informed by outputs of components (1), (2) and (4).
Component 4: Based on an intensive review of the literature on biodiversity from the continental shelf of the focal region, this activity will produce a geospatial data bank on the occurrence, distribution, and abundance of benthic and pelagic organisms to establish a baseline of the biodiversity. The information will be presented in the body of the report as a discussion of each biological group, in addition to figures, maps and tables. Spreadsheets with data on the biological groups surveyed should be included as annexes, as well as general maps of their occurrence and distribution. The information must also be made available in geodatabase format (mdb), containing vector data in shapefile format (shp, shx and dbf) delivered in digital media.
Component 5: It must present a survey of public policy instruments (policies, plans and programs) as well as the relevant legislation (applicable international treaties and infralegal devices such as ordinances, resolutions, normative instructions etc.) that have an interface with the possible development of the activity of wind generation on the continental shelf of the focal area. After gathering all this information, a critical and integrated analysis of how this economic activity could develop in the region will be presented, generating the least possible interference on biodiversity and other current and future uses of the marine space in question. For this purpose, Marine Spatial Planning (MSP) methodologies will be applied, especially the one adopted by the International Oceanographic Commission of UNESCO.

Spreadsheets with the collected data must be attached, as well as general maps of their occurrence and distribution. The information must also be made available in geodatabase format (mdb) containing vector data in shapefile format (shp, shx and dbf) delivered in digital media.

Preliminary results: The development of the project advanced in Component 1, in the selection of countries to review legislation related to the process of Environmental Impact Assessment, marine spatial planning. The countries selected were: China, the United Kingdom, the United States, Australia and the Netherlands. The criteria for selecting countries were: the installed capacity of offshore wind energy, the existence of expansion targets for this type of project in the coming years, and the existence of a consolidated environmental impact assessment system. In addition, related to component 4, the literature review aimed at mapping data on biodiversity on the continental shelf was also started, with a focus on areas in the states of Rio de Janeiro and Ceará.

Preliminary conclusions: Due to the small number of results produced to date and their Preliminary nature, it is not possible to draw conclusions at this time.

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Abstract Title: Municipal Solid Waste Potential for Hydrogen Production in the Sao Paulo State

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Abstract: Hydrogen has gained attention as a sustainable and efficient energy source due to its carbon-neutral nature and low greenhouse gas emissions. However, the majority of hydrogen is currently produced by the petrochemical industry, which is environmentally harmful. This article highlights the potential of using non-recyclable municipal solid waste as a source of hydrogen production, thereby contributing to sustainable energy systems. The focus is on estimating the hydrogen production potential in the Sao Paulo state through the reforming of biomethane from municipal solid waste and the gasification of refuse-derived fuel. This suggests that utilizing these waste materials can play a crucial role in producing clean energy resources and addressing the global problem of waste disposal.

Keywords: Refuse-derived fuel, hydrogen, municipal solid waste.

Introduction and Objectives: Currently, the global energy system depends on a finite supply

from fossil fuels, it is becoming increasingly difficult and costly to extract, putting the security of country's energy at risk. In this way, in recent years, global authorities have been looking for to invest in efficient and sustainable renewable sources to reduce dependence on fossil fuels, and the possible environmental effects caused by their use, diversifying the energy matrix. The interest in hydrogen as an energy carrier is growing, due to it is a sustainable and efficient energy source, a carbon neutral source with low greenhouse gas (GHG) emissions. Hydrogen can be produced from a variety of biomass resources, biomass waste, biofuels (ethanol), municipal solid waste, solar, nuclear and wind energy, however currently most hydrogen is produced from fossil fuels, especially natural gas. The production of hydrogen has several routes, and the route choice of route depends on several factors, such as availability of resources, inputs cost, existing infrastructure and local demand. The growing volumes of non-recyclable municipal solid waste (MSW) that cause problems worldwide can be reused to produce a portion of the world's clean energy resources, becoming important contributors to sustainable energy systems. Recently, biomethane from MSW and gasification of refuse derived fuel (RDF) have received considerable attention, as they offer the alternative of producing hydrogen.

Biomethane can be an alternative feedstock to conventional steam reforming technology, is similar to natural gas and includes additional benefits such as being a renewable resource and reducing greenhouse gas (GHG) emissions by preventing the release of methane into the atmosphere. Waste gasification involves converting the raw material into combustible gases (H2, CO, CO2, CH4 and hydrocarbons) under high temperature and sub-stoichiometric conditions (amount of oxygen below the stoichiometric amount) facilitating the introduction of water vapor as a gasification agent. The formation of organochlorine compounds (dioxins and furans) in gasification is almost negligible and the cleaning system is significantly simpler. In this context, this article presents the potential of MSW for hydrogen production in the state of Sao Paulo, considering biomethane reforming and RDF gasification technologies.

Methodology: This paper presents an estimate of the potential for hydrogen production in the Sao Paulo state from biomethane reforming and fluidized bed gasification of RDF processes, based on research data on waste generation per capita, number of inhabitants per municipality, and treatment capacity of the technologies available in the country. The MSW gravimetric composition for each municipality was assumed equal to the average composition of the region in which it is located in the country. In order to quantify the generation of methane (CH4) from the waste disposal in landfills in each municipality, the methodology of the Intergovernmental Panel on Climate Change (IPCC) "Guidelines for National Greenhouse Gas Inventories" was adopted. On the other hand, in the case of gasification, the municipalities of medium size ($60{,}000 \leq$ inhab $\leq 1000{,}000$) were evaluated.

The analysis was carried out based on two scenarios: the first scenario covers the study of the hydrogen potential according to the current MSW treatment conditions in the Sao Paulo state, i.e., waste collection coverage of 98% and a recyclables recovery rate of 2.2%. The second scenario considers the goals of the national solid waste plan for 2040, a collection coverage of 100% and a recyclable material recovery rate of 20%.

Preliminary results: The Preliminary results shows that the Sao Paulo state has a potential for hydrogen generation from biomethane reforming of 83 thousand t.year-1 and 52 thousand t.year-1 from the RDF gasification. The hydrogen production, according to the goals of the national solid waste plan for 2040, shows that the biomethane reforming process will have a potential of 59 thousand t.year-1 and 37 thousand t.year-1 from the RDF gasification.

Preliminary conclusions: Aiming at sustainable economic development through massive decarbonization, increasing the participation of bioproducts, as well as valorizing MSW as a raw material for other destinations, the São Paulo state presents an attractive market that could be an opportunity for the development of several technologies as well as the study of little explored sources for hydrogen generation. MSW recovery where industry by-products can be sent back into the economy in a circular, low-carbon manner while protecting the basic principles of waste management (waste hierarchy) will be key in the energy transition.

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Abstract Title: Adsorption study of H3BO3 in graphene: a computational approach

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Abstract: Boron is an essential nutrient for plant growth and animals. However, the excess of boron might be hazardous. In an environment rich in water, boron reacts with water forming boric acid (H3BO3). Since boron is found at high concentrations in produced water, there is a need to efficiently perform boric acid filtration for environmental needs, human and agricultural consumption. A promising material for filtration is graphene, since it has good mechanical properties and chemical stability. In order to investigate boric acid filtration through graphene by molecular simulations, such as molecular dynamics and Monte Carlo, we tested how accurate the current description of the interaction between boric acid and graphene is. This test was performed by comparing the interaction obtained from Lorentz- Berthelot (LB) using force fields available in the literature to Density Functional Theory (DFT) calculations with electronic

dispersion. The DFT calculations were performed in the SIESTA code using the KBM functional, while the interaction from LB was obtained in LAMMPS software. The results from DFT show the adsorption energy of boric acid on graphene is 0.4 eV, indicating a relatively strong attraction. Moreover, the results also indicate that LB underestimates the interaction energy, suggesting that its use in molecular dynamics simulations for boric acid filtration through carbon nanostructures might produce unrealistic results. Because of that, we performed a new parametrization of a Lennard-Jones potential based on energies and forces from the DFT calculations in order to obtain a better description of the system of interest. The new potential shows good agreement with DFT results, which indicates that its use in molecular simulations might improve the descriptions of the simulations. With this new potential, molecular dynamics simulations were performed to obtain the profile density of a solution of boric acid adsorption on graphene. The results show that boric acid molecules tend to be adsorbed on graphene, suggesting that this nanomaterial can filter it from water.

Keywords: Boric Acid, DFT, Molecular Dynamics.

Introduction and Objectives: Boron is an essential micronutrient for plant growth and development, and several clinical aspects are related to its insufficiency. However, B excess is also hazardous, even more dangerous than deficiency. Besides, it is used in a wide range of industrial branches, and it is expected that by 2027 mineral and solvent B market will have a revenue of 4.5 billion dollars.1 In an aqueous environment, boron can assume the form of several borates according to the solution pH. In pH 7, boric acid (H3BO3) is the main species present, forming H2BO3-, B(OH)4-, HBO2, and other species in an alkaline environment. Boric acid presents boron on sp2 hybridization, with a pure pz orbital empty. The electroneutrality of H3BO3 makes the behavior of this species very different from those of ions occurring in the feedstock water, requiring specific attention in water purification processes. As water demands tend to grow in the following decades as well as the need for food, the application of desalinated water in agriculture is undoubtedly an alternative. The B concentration in the ocean, the main source of this element, ranges from 0.5 to ppm while in groundwater it ranges from 0.3 to 100 ppm.2,3 To be employed in agriculture, B must reach certain limits according to the demands of each crop, with a tolerable limit of 1 ppm. 4 In addition, the reverse osmosis membranes, which present efficiencies superior to 99.7 % for salts, can remove around 92 % of boron, being unable to reach the optimum parameters for irrigation in some scenarios3. Graphene derivatives, such as pristine graphene, graphene oxide, and reduced graphene oxide present a huge population of pure sp2 carbon atoms, with delocalized electrons dispersed over a cloud that extends through the surface of these bi-dimensional materials.5 Due to the presence of the cloud, these materials have been studied for the adsorption of several species, such as proteins and ions.6,7 As H3BO3 presents B on sp2 hybridization, one might expect the interaction of the empty p orbital with the electron cloud on graphene derivatives to be thermodynamically favourable, allowing for the application of such materials to be employed on the removal of boric acid by adsorption. Besides, the -

stacking is also a constant when dealing with graphene derivatives, leading to the formation of bundles containing multiple sheets. To evaluate the viability of the application of graphene derivatives as adsorbents of boric acid in an aqueous environment, both molecular dynamics simulations at room temperature and calorimetry experiments to obtain the adsorption properties were performed. To accurately describe the interactions of boric acid and graphene, a new Lennard-Jones potential, derived from DFT-KBM calculations, was first parameterized. With this potential, the profile density of a boric acid solution adsorbed on graphene was obtained. This result shows that boric acid is favourably absorbed in graphene.

Methodology: To correctly describe the adsorption properties of graphene towards boric acid using molecular dynamics, it is necessary to use a force field that can accurately describe the interactions between these species. To that end, we first evaluate how well Lorentz-Berthelot (LB) combination rules can describe the potential energy surface compared to DFT calculations. The LB combination rules are approximations widely used when there is no available FF dedicated for specific cross-interactions and are known to be imprecise in certain situations. To compare the interaction energies from LB and DFT calculations, we obtained the potential energy surfaces by calculating the potential energy as a function of the distance between the boric acid and graphene. The interaction energy from LB was obtained within the LAMMPS software. The interaction energies were obtained at 4 different adsorption sites and compared to results obtained through force fields available in the literature using Lorentz-Berthelot (LB) combination rules. The calculations were performed using the SIESTA code and the van der Waals functional KBM as van der Waals forces play an important role in adsorption properties and should be accurately described. To have a fair comparison, the atomic configurations were the same as used in the previous part.

Fitting procedure

As the results for the interaction energy from DFT calculations were significantly different from those currently used force fields, a parametrization for new Lennard-Jones (LJ) potentials to describe the interaction between boric acid and graphene was performed. One LJ potential was selected for each pairwise interaction of each atom present in the boric acid molecule (B, O, and H) and carbon in graphene. In the parametrization process, the error function to be minimized was the squared error of the energy predicted by the new force field concerning the DFT calculations. Only two potential energy surfaces (PES) were selected to perform the parameterization. We used the other two PES, to perform a validation test.

Molecular Dynamics Simulations

With the proposed force field, MD simulation was performed to understand the adsorption properties of graphene towards boric acid. After an energy minimization, the simulation started with phase equilibration and then, a production phase consisted of a 4.00 ns long simulation at NPT. We saved the atomic positions and used them to obtain the profile density of the system. The aimed temperature and pressure were 300.0 K and 1.0 atm, respectively. The timestep used

was 0.50 fs and the radius cutoff for the non-bonded interactions was 14.0 Å.

Preliminary results: Development of Lennard-Jones potential

The results from DFT indicate that the minimum of the energy curve is -0.47 eV (-46,686 KJ mol-1), which is close to what can be considered a chemisorption (-0.5 eV).8,9 Figure 3 A presents the potential energy surface obtained using Lorentz-Berthelot combination rules and DFT - KBM calculations. However, it is worth mentioning that van der Waals functionals, such as KBM, are known to overestimate the adsorption energies. Nonetheless, the results suggest a relatively strong interaction, indicating that graphene might act as an adsorbent for boric acid. Indeed, carbon nanomaterials, such as graphene and carbon nanotubes, for instance, are used for pollutant removal (such as metal íons and polyphenols) in water since they are adsorbent for these materials. The data obtained here suggest that boric acid can also be adsorbed in graphene-like species. The divergence between the potential energy curves for interactions between boric acid and graphene from DFT and current force fields, presented in Figure 3-A, indicates that the latter underestimates the interaction energy. Since the prediction of molecular simulations is dependent on the chosen FF, the results suggest that the current force field might not be appropriate for simulating the adsorption of boric acid on carbon nanomaterials. Thus, there was a need to go beyond Lorentz-Berthelot combination rules by parametrizing a new set of Lennard-Jones potential.

With our results for the PES for two different configurations obtained from DFT and our proposed force field. The proposed force field shows good agreement with the DFT data, indicating that it can reproduce the interactions between graphene and boric acid even in configurations not used in the fitting procedure. It is also worth mentioning that it is known that Lorentz-Berthelot combination rules might not be enough to reproduce the cross-interactions, since it is only a mean approximation, and this might affect the prediction of the thermodynamic properties from molecular simulations. 19 Molecular dynamics of the adsorption process.

With the proposed potential, molecular dynamics simulations were performed to understand the absorption properties of graphene towards boric acid in an aqueous environment. Figure 4 shows the profile density of the system. The boric acid molecules tend to get absorbed on the graphene sheet at its first absorption layer (Langmuir model).

Preliminary conclusions: Due to the fact that boron is found at high concentrations in produced water, as in boric acid, there is a necessity to filter it for human and agricultural consumption. A promising material for filtration is graphene, since it has good mechanical properties and chemical stability. To investigate the performance of graphene as adsorbent of boric acid in molecular simulations, we tested how accurate the current description of the interaction between boric acid and graphene is. This test indicates that LB underestimates the interaction energy, suggesting that its use in molecular dynamics simulations for boric acid filtration through carbon nanostructures might produce unrealistic results. Because of that, we performed a new parametrization of a Lennard-Jones potential for the interactions between boric acid and graphene. With this new potential, simulations were performed to understand the

adsorption process of boric acid adsorption on graphene. The results suggest that boric acid molecules can be adsorbed on graphene, indicating that this carbon nanomaterial might be used for filtrating boric acid from water.

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Abstract Title: Potential for electricity generation from sustainable forest management residues in Brazilian isolated systems

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Abstract: This study emphasises the strategic importance of utilising forest biomass to generate electrical energy in Brazil. This highlights factors such as high forest productivity, sustainable management practices, and timber industry waste. The shift from unsustainable to sustainable forest practices has been underscored, providing both economic and environmental advantages. This paper discusses the prevalence of diesel generation in Brazil's remote areas and the potential of renewable energy sources, particularly biomass. It also addresses the environmental advantages of biomass use and its synergy with sanitation. The main goal of this study was to determine the energy potential of forest biomass waste, particularly in the Amazon region, from commercial wood extraction and FSC-certified sawmills. The methodology estimates the electricity generation potential from timber waste, showing a significant capacity for renewable energy production. The results are expected to contribute significantly to utilising timber waste for energy, meeting energy needs in isolated areas, promoting a shift towards renewable energy sources, reducing greenhouse gas emissions, and supporting sustainable development.

Keywords: Forest biomass; Amazon region; Sustainable Forest management; Sustainability; Renewable energy.

Introduction and Objectives: The generation of electrical energy from forest biomass in Brazil can be considered strategic because of several factors, including high forest productivity, extensive areas available for sustainable and low impact management, a large volume of waste generated in the timber industry, and the commercial availability of modern and efficient conversion technologies.

For a long time, the use of forest products has been associated with deforestation, as their

extraction activities have been carried out without concern for sustainability. However, with the implementation of good forest management practices, which include reduced-impact harvesting techniques aimed at maintaining the ecological, social, and economic functions of forests, it is now possible to generate income while benefiting from the preservation and conservation of natural resources. Brazil has an extensive transmission network known as the National Interconnected System (SIN; Portuguese acronym), which connects power generation to consumption. However, approximately 250 locations are not connected to the SIN for technical or economic reasons. These areas are referred to as Isolated Systems and are primarily concentrated in the Legal Amazon states. To ensure the supply of electrical energy in these isolated systems, each relies on a power plant, with diesel generation being the predominant source. Currently, there is diversification in the Brazilian electrical matrix with the recent increase in the participation of photovoltaic solar and wind energy projects. However, diesel generation still prevails in the isolated systems. The Energy Research Office (EPE; Portuguese acronym) estimated that in 2018, these isolated systems consumed approximately 800,000 m3 of diesel oil, resulting in direct emissions of approximately 2.1 million tons of CO2. It is crucial to identify the potential use of renewable sources in isolated Brazilian systems, specifically for bioenergy. This involves considering 251 isolated systems in the country and EPE's study base, mapping the available renewable resources in each location, and addressing technical, economic, and socio-environmental challenges in the use of these resources while proposing solutions. Consequently, the inclusion of biomass energy generation projects is opportune, especially because of their dispatchable nature and significant contribution to meeting the needs of electrical energy supply and system regulation. The primary aim was to determine the energy potential of forest biomass waste derived from commercial wood extraction in Sustainable Forest Management Plans (SFMPs) and wood processing in sawmills duly certified by the Forest Stewardship Council (FSC) in the Amazon region. This effort was directed towards meeting the demand for electrical energy in Brazil's isolated systems.

Methodology: The methodology used in this study is based on estimating both the theoretical and technical potentials for combined heat and power generation from timber waste in sawmills and forest management harvesting residues in municipalities within isolated Brazilian systems.

Preliminary results: For wood processing waste in sawmills, the estimated electricity generation potential is 133,930 MWh/year, with available electrical power of approximately 19.11 MW. In contrast, the potential for electricity generation from forest management harvesting residues resulted in a total of 600,812 MWh/year and available electrical power of approximately 85.73 MW.

Preliminary conclusions: Apart from its substantial energy potential, which is crucial for distributed generation, sustainable forest production techniques and the utilisation of biomass waste offer environmental benefits because of their renewable nature as well as economic and social advantages. The use of waste helps to address environmental issues by reducing methane emissions from the decomposition of organic matter in biomass derived from forestry and

industrial operations. Additionally, it contributes to emission reduction by replacing fossil fuels in electricity generation in isolated systems. It is also important to highlight the significant synergy between this approach and basic sanitation, as it contributes to the proper disposal of waste, especially urban and rural waste, and provides a sustainable and viable option for their use. However, there are still numerous barriers, primarily economic barriers, that hinder their large-scale implementation. It is anticipated that the results obtained from this forest biomass potential assessment will significantly contribute to the large-scale development of energy utilisation from timber waste, addressing the demand for electrical energy in the country's isolated systems. Moreover, it will foster the transformation of the national electrical matrix towards renewable sources, ultimately resulting in a reduction in greenhouse gas emissions. This transformation involves the substitution of fossil fuels used for energy generation in areas not connected to the SIN while ensuring a stable supply of electrical energy to the studied communities.

Geovanna Paulino Pereira
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Abstract Title: Winds of the Future: Multidimensional Assessment of Socio-Environmental Impacts in Offshore Wind Farms.

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Abstract: Due to the increasing demand for renewable energy sources, offshore wind farms sound like a promising option to meet this growing need, playing a crucial role in mitigating climate change and in the global transition to a more sustainable energy matrix in line with the United Nations Sustainable Development Goals (SDGs). However, the installation of wind farms raises important concerns that transcend engineering and energy boundaries and, therefore, it is necessary to analyse the environmental, social and economic impacts faced in the construction and operation of offshore wind farms. Therefore, from a multidimensional lens, this project will be dedicated to examining the direct and indirect impacts that these developments have on coastal communities. Ultimately, it is expected that this research will not

only expand existing knowledge on the challenges and socio-environmental impacts of offshore wind farms, but also promote a more holistic and balanced understanding of these projects, aligning with the UN SDGs, economic consequences, the sustainable energy transition, the preservation of coastal ecosystems and the well-being of local communities.

Keywords: Wind Energy; Offshore Wind; Wind Farms; Environmental Impacts; Social Impacts and Renewable Energy.

Introduction and Objectives: Wind energy has become a protagonist in the search for clean and sustainable energy sources. The search for renewable energy is aligned with goals 7 – Clean and Affordable Energy, 9 – Industry, Innovation and Infrastructure, 13 – Action against Global Climate Change and 14 – Life in Water of the United Nations. The transition from onshore wind energy to offshore wind energy has been expanding significantly around the world, giving it the potential to play an important role in ensuring energy supply in line with the country's commitments. The modification of the landscape due to the presence of wind turbines can result in the financial devaluation of the area in which it is located. Noise pollution caused by these wind turbines, which generate two types of noise, can contribute to the worsening of this situation. The fauna and flora present at the site may be affected as a result of disturbances caused by the installation of wind farms.
This scientific Initiation research will focus on carrying out a comprehensive review of the impacts on coastal communities. The research will contribute to the compilation and synthesis of current knowledge on the topic. This critical review will be essential to support the multidimensional qualitative analysis of impacts. It can provide a basis for developing more effective assessment and mitigation strategies.

Objectives: This project's main objective is to collaborate with the carrying out of a comprehensive and holistic multidimensional study to evaluate the socio-environmental impacts arising from the establishment of offshore wind farms, seeking to focus on two impacts that will be identified during the analysis of the causal chain, aiming to contribute to the responsible development of this form of renewable energy, balancing environmental sustainability, the well-being of coastal communities and regulatory compliance. Specific objective 1: Align this research proposal with the other individual projects of the project “Assessment of the environmental and social impact of harnessing offshore wind energy ("EnvSoOff")” in order to identify synergies and opportunities for collaboration; Specific objective 2: Comprehensively review the state of scientific and technical art regarding the impact assessment of the installation of offshore wind energy parks and their impact on the region in which it is located; Specific objective 3: Conduct a qualitative analysis of the collected data, with the purpose of exploring the complex interactions between the environmental and social impacts of offshore wind farms. This qualitative analysis will allow for the identification of nuances and insights that may not be captured by quantitative methods alone. This will contribute to a more complete view of the implications related to the implementation of these wind farms; Specific objective 4: Select two impacts to focus on causal chains and develop

reports reporting key evidence.

Methodology: A systematic review is a research method that involves the search, selection and critical analysis of relevant studies on a given topic, in a systematic and transparent way. Carrying out systematic reviews follows established guidelines, such as those proposed by PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses. In this way, this research project will employ a systematic review as part of its methodology. This means that it will follow a rigorous and pre-established protocol to identify, select and critically analyze relevant studies on the multidimensional impacts caused by the implementation of offshore wind farms, consolidating and synthesizing existing knowledge on the topic. This approach, aligned with the guidelines established by the scientific community, ensures that the review process is conducted in a transparent, objective and judicious manner, providing reliable and robust results to contribute significantly to the field of study in question. The research will be carried out in the main scientific databases such as Dedalus (USP), Web of Science, Scielo, Google Scholar, Sciencedirect and other renowned databases. The keywords used will be wind energy, offshore wind energy, wind farms, environmental impacts, social impacts and renewable energy. The search will be carried out in Portuguese and English.

Preliminary results: There are no Preliminary results yet.

Preliminary conclusions: There are no Preliminary conclusions yet.

Guilherme de Aquino Fernandes Sousa
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Abstract Title: How far has the low-carbon energy transition contributed to energy poverty and social exclusion? Analysis from the Brazilian context

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Abstract: Guaranteeing the distribution of affordable, reliable and sustainable energy is a major challenge for most developing countries. An unequal and insufficient distribution of energy resources can harm economic development and the quality of living among the population. However, considering the current climate emergency, tackling this problem might have to be accompanied by decarbonization and energy transition. In the case of Brazil, the necessity to meet the energy demands of the broad population, especially the lower income, often surpasses the need to reduce carbon dioxide emissions. Therefore, expanding the renewable energy production is not always a viable solution considering the economic and technological

limitations that some regions face. The aim of this study is to analyse the duality that energy transition can represent in policy making by considering the effects on the cost of electricity for the consumer, the liability of the power grid and the cost of implementation and maintenance.

Keywords: Energy Transition, Energy Poverty, Renewable Energy, Brazil.

Introduction and Objectives: The energy transition into a low carbon economy demands a broad effort that includes a change in social perception, a shift in public policies, technological improvements and economic reconfiguration. Remarkably, the consequences of such a paradigm shift on the conditions of energy poverty and exclusion are not yet fully understood and represents an important object of study considering the current state of the climate crisis. In Brazil, the cost of electricity bills takes up at least half of the income in 46% of the households (IPEC, 2022), and increases on this cost can push millions of people into food insecurity. The importance of taking into account how the expansion of renewable energies affects the cost of electricity to the consumer is vital to guarantee the affordability of energy. In this regard, this study aims to analyze the duality that energy transition can represent in policy making by considering the effects on the cost of electricity for the consumer, the liability of the power grid and the cost of implementation and maintenance.

Methodology: The quantitative and qualitative data analysis were made using data of electricity consumption collected from databases available in the National Electrical Energy Conservation Program (ProcelINFO) and the Energy Research Office (EPE).

Preliminary results: The data shown by the Ten-Year Energy Expansion Plan 2031 (PDE, 2031) demonstrates that the increase of the share of renewable energies in the power grid might encounter adversity regarding the cost of implementation and maintenance of new technologies, which can translate into higher costs to the consumers. It is expected that the growing demand of energy will outpacetechnological advances in renewable energy. The ongoing study will provide an analysis of the trends in demands for energy and the cost of renewable energy.

Preliminary conclusions: The discussion of energy poverty gained relevance with the growing necessity to transition into a greener future. The analysis of the situation of distribution of energy to the lower income populations is shown to be ever more important considering the direct correlation between energy consumption and well-being in modern times. The great number of people in Brazil whose survival relies on the stable supply of energy saves little space for mistakes in public policy that can affect the cost of electricity. In this regard, this study sought to deepen the discussion on the effects the necessity of energy expansion on energy poverty reduction.

Energy Transition
RESEARCH & INNOVATION

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Abstract Title: Integration of Photovoltaic Energy in Urban Planning: Promoting resilience and decarbonization of cities through solar neighbourhoods

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Abstract: Growing global urbanization and dependence on fossil fuels are two of the main challenges facing cities today. Photovoltaic energy is one of the sustainable and renewable alternatives that can be used to overcome these challenges. This article discusses the integration of photovoltaic energy in new urban planning through solar neighbourhoods collaborating with urban resilience and decarbonization of cities. The study presents examples of solar neighbourhoods in different parts of the world that have been effective in producing electricity through photovoltaic panels integrated into residential and commercial buildings. These solar neighbourhoods also led to a reduction in greenhouse gas emissions, contributing to the improvement of air quality in cities.
Furthermore, the article explores urban planning strategies that can be used to facilitate the integration of photovoltaics into solar neighbourhoods. These strategies include tax incentives, specific legislation, public policies and partnerships with renewable energy companies. Finally, the article highlights the importance of urban resilience in the context of integrating photovoltaic energy into urban planning. Urban resilience is an approach that seeks to make cities more adaptable and resilient to extreme events such as climate change and natural disasters. The integration of photovoltaic energy in solar neighbourhoods can contribute to increase urban resilience, independence from fossil fuels and energy security in cities. In conclusion, the integration of photovoltaics into urban planning through solar neighbourhoods can be an effective strategy to promote resilience and decarbonization of cities. However, commitment from government authorities, businesses and local communities is needed to implement this change.

Keywords: photovoltaic energy, urban planning, urban resilience, decarbonization, solar neighbourhoods.

Introduction and Objectives: The rapid growth of global urbanization and increasing dependence on fossil fuels pose daunting challenges for cities around the world. Climate change and environmental degradation have resulted from these unsustainable development patterns, and we now need to develop innovative and effective solutions to promote urban resilience and decarbonization. In this context, the integration of photovoltaics into urban planning through solar neighbourhoods emerges as a promising approach to address these challenges in a sustainable way. According to the Brazilian Association of Photovoltaic Solar Energy

(ABSOLAR), photovoltaic solar energy has shown significant growth in Brazil and worldwide. By 2021, installed photovoltaic solar energy capacity in Brazil surpassed the 10 gigawatts (GW) mark, representing an increase of more than 500 times compared to 2012. Globally, photovoltaic capacity consumed more than 770 GW in the same period.

Photovoltaic energy, which converts sunlight into electricity, presents itself as a sustainable and renewable alternative to meet the energy needs of cities. Through the installation of solar panels on residential and commercial buildings, parking lots and public spaces, solar neighbourhoods have the potential to become self-sufficient sources of clean energy.

In addition to promoting urban resilience, photovoltaic energy contributes to the decarbonization of cities. According to the International Renewable Energy Agency (IRENA), photovoltaic solar energy can avoid the emission of up to 2.5 gigatons of carbon dioxide (CO2) per year by 2050, if there is a significant increase in its implementation. This represents a significant reduction in greenhouse gas emissions, helping to mitigate the effects of climate change. By promoting urban resilience, solar neighbourhoods can contribute to reducing the vulnerability of cities to extreme weather events and continuous energy supply. The diversification of energy sources and the local generation of electricity provide greater energy security and minimize the impacts of events such as storms, floods or failures in the electrical grid. In addition, the integration of photovoltaics reduces dependence on fossil fuels, greenhouse gas emissions and pollutants in the environment. To facilitate the integration of photovoltaic energy in urban areas through solar neighbourhoods, several urban planning strategies can be adopted. According to ABSOLAR, the implementation of public policies, with According to specific laws and regulations, it can encourage the use of photovoltaic solar energy in residential and commercial buildings and public spaces. Additionally, tax incentives such as tax exemptions or reductions can make solar energy more affordable and attractive to residents. Partnerships with renewable energy companies are also essential to provide the technical knowledge, financial resources and infrastructure necessary for the installation and maintenance of photovoltaic systems.

By exploring these aspects, this article seeks to provide a comprehensive view on the integration of photovoltaics in urban planning through solar neighbourhoods, highlighting their contributions to the resilience and decarbonization of cities. Based on current data from ABSOLAR and other relevant sources, it is expected that the presented results can contribute to a deeper understanding of this sustainable approach and inspire the adoption of urban policies and strategies that promote a cleaner, more resilient and environmentally conscious energy future.

Objectives: The main objective of this study is to investigate the integration of photovoltaic energy in urban planning through solar neighbourhoods and to analyse its impacts on promoting resilience and decarbonization of cities. We intend to examine the benefits and challenges of this approach, as well as identify planning strategies and public policies that can facilitate its effective implementation. In addition to the main objective, this study also seeks to achieve the following objectives: Present real examples of solar neighbourhoods in different parts of the

world to identify their characteristics, benefits and lessons learned. Investigate the role of photovoltaic energy in promoting energy self-sufficiency in solar neighbourhoods, encouraging the adoption of renewable sources and strengthening energy security in cities. Evaluate the impact of integrating photovoltaic energy into solar neighbourhoods in reducing greenhouse gas emissions and combating climate change. Investigate the advantages of implementing solar neighbourhoods, such as creating local jobs and reducing energy costs for residents.

Justification: This study is justified by the urgency of finding efficient solutions to the challenges faced by cities in relation to urbanization, energy resilience and decarbonization. The integration of photovoltaic energy in urban planning through solar neighbourhoods emerges as an innovative approach, capable of addressing these issues simultaneously. By investigating the integration of photovoltaics in solar neighbourhoods, this study could contribute to the generation of knowledge about the benefits and challenges of this approach, providing information for decision-making by government authorities, companies and local communities. Furthermore, this study has the potential to stimulate the development of more effective public policies and sustainability oriented urban planning strategies.

Methodology: To achieve the proposed objectives, this study will follow a mixed methodological approach, combining qualitative and quantitative analysis. A systematic review of the literature will be carried out to gather relevant information about the integration of photovoltaics in urban planning and its effects. To obtain a deeper understanding, several sources were consulted, including reports, articles, news and materials, as well as several webinars held and available online, adding new ways of research through the technological advances of recent times.

Case studies and real examples of solar neighbourhoods will be analysed to identify their characteristics, benefits and challenges. Quantitative data, such as installed photovoltaic energy capacity and reduction of greenhouse gas emissions, will be collected from voluntary sources, such as official reports, specialized organizations and granted databases.

Interviews and surveys were conducted with experts, government officials, representatives of the renewable energy industry and members of local communities to gain additional perspectives on the implementation of solar neighbourhoods and their guidelines.

The analysis of the collected data will be carried out systematically, using qualitative content analysis methods and neighbourhood references to identify trends, patterns and results.

By adopting this methodological approach, we seek to gain an understanding of the integration of photovoltaics in urban planning through solar neighbourhoods, contributing to the construction of a more specific knowledge on this issue.

Preliminary results: The results presented in this article demonstrate the positive potential of integrating photovoltaic energy into urban planning through solar neighbourhoods. Solar neighbourhoods can significantly contribute to the resilience and decarbonization of cities, providing energy and environmental benefits. The examples presented proved capable of achieving energy self-sufficiency, producing enough electricity to meet the needs of their

residential and commercial buildings. This reduces reliance on traditional energy sources and strengthens the neighbourhood's energy security. In addition, the implementation of Solar Neighbourhoods tends to present a reduction in greenhouse gas emissions. Photovoltaic solar energy is a clean energy source, eliminating or minimizing the carbon emissions associated with generating electricity from fossil fuels. In this way, solar neighbourhoods contribute to the decarbonization of cities, helping to combat climate change.

In terms and in economic terms, the implementation of solar neighbourhoods, such as those presented here, can stimulate the local economy. The installation, maintenance and operation of photovoltaic systems generate direct and indirect jobs, contributing to the economic growth of the region. Furthermore, the reduction in energy costs provided by solar power generation benefits neighbourhood residents by providing long-term financial savings. However, it is important to emphasize that the integration of photovoltaics in solar neighbourhoods presents challenges. Such challenges can be overcome with government incentives, such as rewards and low-interest lines of credit, and adapting existing infrastructure to accommodate solar power.

In summary, the results show that the integration of photovoltaics into urban planning through solar neighbourhoods can bring concrete benefits to cities, promoting resilience, decarbonization and economic growth. Although the analysis of these results is preliminary and of international projects, they provide a positive and promising perspective for the adoption of solar neighbourhoods in the national territory as part of a comprehensive strategy for a more sustainable energy future.

Preliminary conclusions: The integration of photovoltaic energy in urban planning through solar neighbourhoods presents itself as an innovative and promising approach to face the challenges of urbanization, resilience and decarbonization of cities. Throughout this article, we explore the benefits and advantages of this integration, as well as the challenges that must be overcome.

The case studies demonstrated that solar neighbourhoods have the potential to promote energy self-sufficiency, reduce greenhouse gas emissions and generate the local economy. In addition, urban resilience is strengthened through local energy generation and reduced dependence on traditional sources, making cities more prepared to face extreme events.

However, it is essential to emphasize that the successful implementation of photovoltaic energy integration requires a joint commitment from government authorities, companies and local communities. It is necessary to establish adequate public policies and financial incentives to facilitate the adoption of solar energy, as well as to invest in the modernization of electrical infrastructure and training of the workforce. The integration of photovoltaics into solar neighbourhoods not only contributes to urban resilience and decarbonization, but also entails social and environmental climate benefits. The generation of clean energy reduces air pollution, improves the quality of life for residents and raises awareness of the importance of sustainability.

As we face global challenges such as climate change mitigation and the search for sustainable energy solutions, integrating photovoltaics into urban planning through solar neighbourhoods emerges as a powerful and viable strategy. This approach drives a necessary energy transition

and brings us closer to more resilient, efficient and environmentally responsible cities. Therefore, it is imperative that government, companies and communities collaborate and promote the implementation of solar neighbourhoods as an integral part of urban development. In doing so, we will be building cities that will be models of resilience and decarbonisation, demonstrating a commitment to a sustainable future for present and future generations. The integration of photovoltaics into urban planning is a significant step towards this goal, driving the transformation of our cities into more efficient, sustainable and resilient urban centres.

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Abstract Title: Optimization study of blue hydrogen distribution as an alternative fuel to diesel in the State of São Paulo

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Abstract: The Brazilian transportation sector emitted 393 Mt of CO2 in 2021, with 49.4% of its energy source being diesel oil. Therefore, decarbonized fuel alternatives such as blue hydrogen (BH2) are increasingly necessary. This initial study aimed to analyse the potential of supplying BH2 to the State of São Paulo. Linear programming was employed to simulate different scenarios of BH2 distribution in the state's administrative regions, using input data consisting of diesel oil demands in each region and the distances between them and a hypothetical production point located in Santos, on the coast of São Paulo. Preliminary results indicate that higher BH2 production leads to an increase in the number of serviced locations. However, the model prioritizes inland regions, which could result in higher transportation costs and the potential economic infeasibility of the modelled system. In this context, this work aims to enrich the model with possible costs associated with BH2 transportation to better understand how the relationship between distances and costs reflects on the modelled distribution system and, consequently, on the viability of blue hydrogen as an alternative fuel to diesel oil in the transportation sector in the State of São Paulo.

Keywords: Blue Hydrogen; Operations Research; State of São Paulo; Diesel Oil; Linear Programming.

Introduction and Objectives: After the trend toward significant global warming predicted in the Sixth Assessment Report of the Intergovernmental Panel on Climate Change, national discussions on reducing greenhouse gases (GHG) emissions have strengthened. In this regard, hydrogen (H2) has been recognized as a possible decarbonization solution for future energy systems. It is considered an alternative to the direct burning of fossil fuels, especially for sectors with challenging emission reductions, such as freight transportation. Among the different technological routes for H2 production, Blue Hydrogen (BH2) stands out as a promising option to drive the development of a low-carbon market. Its production is carried out through Steam Methane Reforming (SMR), in which hydrogen atoms contained in methane (CH4) and water vapor (H2O) molecules are extracted, while residual carbon and oxygen combine to form carbon dioxide (CO2). Subsequently, CO2 is captured and can be used by various industries (e.g., carbonation of beverages, dry ice manufacturing, and cryogenic food preservation) or even stored in geological reservoirs. This process is called Carbon Capture, Utilization, and Storage (CCUS). In the transportation sector, CO2 emissions from the burning of fossil fuels totaled approximately 393 Mt in 2021, with approximately 107 Mt (over 25%) originating from the freight transportation sector in the same year. Additionally, during the same period, 49.4% of the sector's energy consumption was represented by diesel, a fuel that generates both human health and environmental impacts after combustion. Furthermore, it is worth noting that the transport sector's share of final energy consumption is expected to be around 32% between 2021 and 2031, with diesel accounting for approximately 51% of the total consumption by the end of this period. According to the National Agency of Petroleum, Natural Gas, and Biofuels, in 2019, Brazil produced about 41 million cubic meters (Mm3) of diesel, with over 30% of this total consumed in the state of São Paulo alone in the same year. Therefore, given the projections of increased energy demands in the coming decades, especially in major global metropolises, conducting simulations, even of a hypothetical nature, plays a crucial role in the process of seeking optimal solutions in transportation system planning. In light of this, the present study aimed to evaluate the potential for substituting diesel with blue hydrogen in the transportation sector of the state of São Paulo using linear programming. It is important to note, however, that the consumption considered in each location does not solely represent the state of São Paulo, as it encompasses vehicles that travel on its roads but have starting and/or destination points in other locations. Moreover, vehicle refueling in the state of São Paulo does not equate to the internal consumption of that state but rather reflects specific demand in the region in question.

Methodology: This work examines the substitution of diesel demand with hydrogen in the different administrative regions (AR) of the State of São Paulo. To do so, a linear programming model was developed to assess the optimal allocation of BH2 capable of meeting the demand of each location. It is assumed, therefore, that the diesel oil consumption in these regions is primarily driven by the cargo and passenger transportation sector (trucks and buses). Furthermore, it is assumed that hydrogen production will take place near the coast of São Paulo,

as the supply of natural gas for BH2 production will come from offshore reserves. Once produced, the hydrogen will be distributed to the interior of the State of São Paulo, according to the scenarios defined below.

1. BH2 Distribution Scenarios

In this study, six scenarios of BH2 distribution were simulated, taking into account different daily production capacities of the hydrogen plant (500, 1000, and 2000 tons) and supply levels, covering half or the entire energy demand of each administrative region relative to diesel consumption. The annual production values were established based on the daily production capacity scenarios used in the EPE study on BH2, including an additional scenario of 2,000 tons per day production to enrich the analysis.

2. Conversion of diesel consumption to equivalent hydrogen

To obtain the quantities of hydrogen required to meet the energy demand for diesel in the RAs, the Lower Heating Value (LHV) of each fuel was used as a conversion factor.

3. Linear Programming

Linear Programming (LP) was employed to optimize hydrogen distribution for meeting regional energy demands efficiently. LP, a mathematical optimization technique developed in the 1940s, uses the Simplex method to address linear constraint problems. LP involves three key components: decision variables, constraints, and an objective function.
Decision variables, denoted as 'x,' correspond to demand points (RAs) and are binary (0 or 1) to signify whether a point receives hydrogen based on availability.
The variable 'y' represents the hydrogen allocation to specific points, ensuring the total allocation does not exceed annual production capacity.
Another constraint is the total resource quantity produced ('R'), determined by the BH2 plant's production capacity (e.g., 500, 1000, or 2000 t). The sum of hydrogen quantities allocated at selected points ($\sum yi$) must not exceed 'R.'
Demand for each point is represented by the variable 'd,'. If a point is selected ('x1 = 1'), hydrogen allocated ('y1') equals the demand ('d1').
Lastly, 'z' is defined as the summation of 'x' values ('z = $\sum xi$') and serves as the model's objective, aiming to maximize the number of satisfied administrative regions' demands with hydrogen.

4. Google Sheets and Solver

To input quantitative data regarding energy demands and various H2 production scenarios, we utilized the Solver add-on integrated with Google Sheets to perform linear programming calculations.

Preliminary results: The model selected points whose sum of equivalent H2 consumption was less than or equal to the total annual production of this input. The locations with the lowest consumption values were prioritized by the model as a strategy to maximize the quantity of RAs supplied. The AR of Santos was chosen as the point of BH2 reception in the six simulated scenarios due to its lower energy demand compared to all the others. This was followed by the

ARs of Barretos, Registro, Ribeirão Preto, Itapeva, Central, São José dos Campos, Sorocaba, Franca, and Presidente Prudente, respectively, in terms of their representativeness levels in the model. Among the simulated scenarios, C5 was the one that encompassed the highest number of ARs, which resulted from the greater availability of BH2 to meet only half of the demands. Scenarios C3 and C6 yielded the same result of z = 6. In these scenarios, there is a proportional relationship: while in C3, 365,000 tons of BH2 are produced to meet 50% of the demand, in C6, twice the amount of BH2 is supplied to meet double the demand. Despite the increased supply of BH2 demands in C6 and the potential scale-up demonstrated by EPE in the production of larger volumes of hydrogen, in this scenario, the chosen locations are farther from Santos, which would result in higher transportation costs for BH2 compared to C3. Furthermore, theoretically, the transportation of BH2 to the Barretos, Araraquara, and Ribeirão Preto administrative regions would cross the São Paulo administrative region, and the sum of the hydrogen volumes in C6 allocated to the three more inland administrative regions (336,534t) would be sufficient to meet the equivalent BH2 demand in São Paulo (324,091t). A similar reasoning is valid for analyzing scenarios C1 and C4. Both presented z = 4, but in C4, the RA Ribeirão Preto was prioritized over Itapeva. This greater distance could also be more costly in terms of transporting BH2. Furthermore, in C4, the sum of the demands of Barretos and Ribeirão Preto (204,760t) is equivalent to an amount of BH2 sufficient to supply Sorocaba (182,353t), which is closer to Santos and, consequently, would generate lower BH2 transportation costs.

Preliminary conclusions: The model presented some limitations: the distances between demand points and production points were not considered; only the quantity of supplied locations was the value to be maximized. Transportation costs were also not added to the model, which could have resulted in different outcomes. Therefore, it is evident that further studies are needed to gain a deeper understanding of the feasibility of BH2 production and its potential as an alternative fuel to diesel. In some scenarios, more distant locations from urban centers were chosen as suitable recipients for BH2. However, their technological and economic constraints may render the implementation of this system unfeasible. Conversely, even though the demands of more populous administrative regions, such as São Paulo, may be substantial, their financial capabilities could overcome the economic challenges associated with BH2 production, transportation, and storage. These locations may be prioritized for receiving hydrogen in a scenario of actual large-scale production. It's worth noting that different production locations can influence the viability of BH2 as a fuel. Producing it within the State of São Paulo, for example, could create a more favourable scenario for supplying energy to inland administrative regions in terms of transportation costs or even for serving larger quantities of administrative regions (maximizing z). Furthermore, in future studies, there is an intention to refine the model with data that encompass various variables related to the effective implementation of BH2 as an alternative fuel, such as distances, costs, and other quantitative data concerning logistical challenges.

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Abstract Title: Life Cycle Assessment (LCA) evaluation of the uses of vinasse produced in the Brazilian sugar-energy sector

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Abstract: Vinasse, a by-product of ethanol production, has been used by sugar-energy plants as fertigation for sugarcane plantations. However, application without proper criteria can cause nutrient imbalance and soil salinization. In addition, the vinasse fertigation process emits greenhouse gases such as methane. To minimize these problems, it is necessary to treat the vinasse before application. Experts suggest anaerobic biodigestion of vinasse and its concentration as best management practices. To identify and quantify the impacts of this use, a Life Cycle Analysis (LCA) study will be carried out considering different scenarios: (i) raw vinasse (fertirrigation), (ii) biodigestion of vinasse, and (iii) biodigestion of vinasse and filter cake. The LCA study will also include the concentration stage of digested vinasse using the electrolytic concentrator under development in project 56 - Potentialities in the Sugar-Alcohol Sector: valorisation of vinasse.

Keywords: LCA, vinasse, sugar-energy sector.

Introduction and Objectives: The sugar and alcohol manufacturing process generate large quantities of residues, including vinasse (at a rate of 10 to 14 m3 of vinasse per m3 of ethanol produced), which can be highly polluting for the environment. Since the 1970s, the discharge of vinasse into bodies of water has been prohibited by legislation, which has made its disposal a challenge due to its high volume. As an alternative, vinasse has been used as a fertilizer on sugar cane plantations, avoiding pollution of water bodies, but it can cause soil salinization problems and contamination of aquifers if not applied correctly. In addition, the process of fertirrigation with vinasse emits greenhouse gases such as methane (CH4) and nitrous oxide (N2O), due to the high levels of organic matter and nitrogen present in vinasse. These gases are emitted during the storage, transportation and application of vinasse (Lisboa et al., 2011; Poveda, 2019). To minimize these negative effects of vinasse application on soil and greenhouse gas emissions, experts recommend the development of better waste management practices, such as: - Anaerobic digestion of vinasse, reducing the organic load and allowing the capture and utilization of biogas produced in the process, thus mitigating methane emissions into the atmosphere; - Integration of anaerobic digestion of vinasse with subsequent

concentration to decrease volume and transportation issues, while also enabling the energy utilization of biogas.

This work aims to conduct a Life Cycle Assessment (LCA) of vinasse uses in the Brazilian sugarcane sector. The LCA is being carried out in three distinct scenarios: Scenario 1 involves fertirrigation with raw vinasse. Scenario 2 involves biodigestion of vinasse with subsequent biogas production and the use of digested vinasse in fertirrigation. Scenario 3 (under development) involves biodigestion of vinasse and filter cake with subsequent biogas production and the use of digested residue in fertirrigation. It is important to note that in Scenarios 2 and 3, the produced biogas is used for electricity generation and biomethane production. An LCA study will also be conducted, including the concentration stage of vinasse in all three analyzed scenarios before its application in sugarcane fertirrigation. The system to be analyzed refers to the electrolytic concentrator of vinasse being developed as part of project 56 from RCGI/USP.

Methodology: As mentioned in the previous section, LCA is being conducted in three distinct scenarios: (i) fertirrigation with raw vinasse; (ii) biodigestion of vinasse with consequent biogas production and use of biodigested vinasse in fertirrigation; and finally (iii) biodigestion of vinasse and filter cake with consequent biogas production and use of the biodigested residue in fertirrigation. In the scenarios 2 and 3, the biogas produced is used for electricity generation and biomethane production. The functional unit adopted in the study was 1 ton of vinasse produced in the distillation tower of the sugarcane mill. Once the objective and scope of the study for current uses of vinasse were defined, the necessary data from the sugarcane industry were analyzed and determined for the application of LCA. After defining the data, the next step was to collect these data. The OpenLCA software was used for conducting the LCA study. The following impact categories were analyzed: Climate Change, Acidification, Eutrophication, Human Toxicity, Terrestrial Ecotoxicity, and Stratospheric Ozone Depletion. The data inputted into the software was obtained from the Life Cycle Inventory (LCI) developed for each scenario, where the inputs and outputs of each analysed system were identified. For the development of scenario 2, two distinct situations were analysed. In the first case, the loss of biogas in the vinasse biodigestion and biogas cleaning processes, as well as the loss of biomethane in the upgrading process, were considered. In the second case, these losses were not taken into account. In scenario 3 is currently under review for data refinement and the inclusion of this data in the OpenLCA software. The results generated by the software will be analysed and interpreted for this specific scenario, according to the selected impact categories, similar to what was done for scenarios 1 and 2 presented earlier. The LCA results of the three analysed scenarios for current uses of vinasse in the sugarcane industry will then be analysed and compared. The next step involves finalizing the LCI of the previously analysed scenarios, including the concentration stage of vinasse in different cases: (i) concentration of raw vinasse, (ii) concentration of biodigested vinasse, and (iii) concentration of biodigested vinasse and filter cake. The LCI quantifies the inputs and outputs of the studied system using the electrolytic concentrator developed within project 56. The data obtained from the LCI, including the

concentration stage, will be inputted into the OpenLCA software for conducting the LCA. The results obtained from these three new scenarios will be analysed and interpreted, considering the selected impact categories mentioned above. Finally, there will be a comparison between all the results from the LCA studies conducted in the project.

Preliminary results: During the project development, preliminary LCA results were obtained using the OpenLCA software and analysed for six environmental impact categories, as mentioned above. The data inputted into the software came from the LCI developed for each scenario, where the inputs and outputs of each analysed system were identified. The following results to Scenarios 1 and 2. Scenario 3 (vinasse biodigestion and filter cake) is currently under review for data refinement and inclusion in the OpenLCA software. In Scenario 1, which involves fertirrigation with raw vinasse, the results showed that the main contributions to environmental impacts are related to Climate Change, with an emission of 31.27 kgCO2eq, and Eutrophication, with a load of 0.79 kg PO43-eq. The other evaluated impacts had lower values. In Scenario 2, which involves vinasse biodigestion with biogas production and the use of the biodigested effluent for fertirrigation, two separate analyses were conducted. The results showed that, considering losses, the main impacts are related to Climate Change, with an emission of 17.04 kgCO2eq, and Eutrophication, with a load of 0.60 kg PO43-eq. Without considering losses, the values were slightly different, but the same impact categories were more significant. As for Scenario 3, which deals with vinasse and filter cake biodigestion, it is currently undergoing data review and refinement. Therefore, the preliminary results obtained from 1 ton of vinasse indicate that, among the analysed impact categories, Scenario 2, which involves vinasse biodigestion (with or without loss of biogas and biomethane to the atmosphere), showed lower impact values in the "Climate Change" and "Eutrophication" categories compared to Scenario 1 (fertirrigation with raw vinasse). Regarding Climate Change, although all processes contribute to this category, the impact was lower in the vinasse biodigestion scenario, mainly due to the avoided CO2eq emissions in the electricity generation system from biogas, as well as zero CO2eq emissions during the transportation and application of biodigested vinasse to the soil (due to the absence of CH4 emissions from biodigested vinasse). The impact was even lower when losses of biogas and biomethane to the atmosphere were not considered.
Regarding Eutrophication, although there are contributions at various stages of the process in the vinasse biodigestion scenario, the use of biodigested vinasse for fertirrigation of sugarcane causes less ecological imbalance compared to using raw vinasse. As for the other impact categories analysed (Acidification, Human Toxicity, Terrestrial Ecotoxicity, and Stratospheric Ozone Depletion), there was no significant difference between the scenarios.

Preliminary conclusions: The preliminary results presented demonstrate that the biodigestion of vinasse can be a sustainable alternative in terms of reducing environmental impacts, especially in the categories of Climate Change and Eutrophication. However, it is important to note that the results of Scenario 3 are still undergoing data review and refinement, which may provide additional information on the environmental impacts associated with vinasse and filter

cake biodigestion.
Furthermore, the study highlights the importance of considering different factors, such as losses of biogas and biomethane, in assessing the environmental impacts associated with vinasse utilization processes. The results obtained from these analyses provide valuable insights for decision-making in the sugarcane industry, contributing to the development of more sustainable strategies in vinasse utilization. It is worth noting that these preliminary results represent an evolving foundation, and future studies will provide a more comprehensive and in-depth analysis, including the electrolytic concentration of vinasse. To this end, a new LCA is being developed for each analysed scenario, with the inclusion of the vinasse concentration stage before its application in sugarcane fertirrigation. This stage refers to the electrolytic concentrator of vinasse, currently being developed in Project 56.

0811 - NBS15 (TV3)

Chairs: Carlos Cerri – Maurício Cherubin

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Escola Superior de Agricultura Luiz de Queiroz (ESALQ/USP)

Abstract Title: Soil carbon storage in Brazilian drylands: status, opportunities and challenges

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Abstract: Integrated agricultural systems have great potential to increase soil organic matter, directly influencing the carbon and nitrogen content of the soil. However, information on the influence of these systems on soil organic carbon (SOC) stock in the Brazilian drylands is still scarce. Therefore, the aim of this study is to perform a meta-analysis to recognize the current state, opportunities, and challenges for carbon storage in agricultural systems in the Brazilian semi-arid region. Carbon stock data were extracted from about 53 articles considering the use of cultivated plants and pasture areas, 28 articles in areas of native Caatinga, and 9 articles in integrated agricultural systems of the Brazilian drylands. In the three types of land use, soil organic carbon stock data were evaluated up to 0.3 meters in depth. Differences in soil carbon stock indicate that integrated agricultural systems have an average of 65 Mg ha-1, followed by native Caatinga with 50 Mg ha-1, and agriculture (including pastures and monoculture) with 27 Mg ha-1. Therefore, the greatest difference observed in soil carbon stock was 38 Mg ha-1 between integrated agricultural systems compared to pasture and monoculture areas. The smallest difference observed in carbon stock was 23 Mg ha-1 between native Caatinga

compared to pasture and monoculture areas. In this way, the adoption of integrated agricultural systems can be considered an opportunity to increase the stock of carbon in the soil. However, several challenges must be considered due to the level of aridity and water availability in the region. In conclusion, the demand for more research to assess the potential of different agricultural systems to store carbon up to one meter deep in the Brazilian semi-arid region is remarkable.

Keywords: Nature-based solutions; Carbon stock; Semiarid.

Introduction and Objectives: The Brazilian drylands region has an area of approximately 1.129.000 km2 (Souza Medeiros et al., 2020) located in the northeast region of Brazil and the north of the state of Minas Gerais, occupying about 12% of the national territory (Althoff et al., 2016). According to Mapbiomas, (2023), the Brazilian drylands, present about 37.4 million hectares (M ha) destined for agriculture and livestock. The use for pasture is about 23 M ha, however, 16.1 M ha (70 %) of the pastures of this biome are in severe and moderate degradation (Mapbiomas, 2023). Therefore, the incentive for the adoption of conservationist practices (IAS for example) can contribute to the increase of the soil carbon storage in the Brazilian dryland region. This work will summarize and synthesize the main differences between studies and sources to provide a comprehensive understanding of the changing soil carbon stock of agricultural systems in the Brazilian semi-arid region. Therefore, the objective of this study is to carry out a literature review to contextualize the current state, opportunities, and challenges for carbon storage in agricultural systems in the Brazilian hinterland.

Methodology: The climate of the Brazilian drylands is classified by Köppen as type BSh, representing a hot and dry semi-arid climate with mean annual rainfall of 800 mm, sunshine approximately 2800 h year−1, annual mean temperatures of 27 °C, evapotranspiration of 2000 mm year−1, air relative humidity of 50% (Althoff et al., 2018), and a dry season varying between 5 and 9 months a year (Maia et al., 2007). Most of the area of the Brazilian dry lands are occupied by natural vegetation (64.7%), corresponding to an approximate area of 73 M ha. On the other hand, agricultural activities, including cultivated areas and animal production, occupy 37.4 M ha (33.2%). The Web of Science - Clarivate Analytics and Scopus Platform database were used to collect the bibliographic data. The search was performed in the month of February 2022, with the help of the "Topic Field", which considers the "Title", "Abstract", and "Keywords plus" of each record. The search was limited to scientific articles and literature reviews. The search terms used in both databases were: ("soil carbon stock*" OR "soil carbon" OR "soil organic") AND ("integrated system*" OR "integrated crop livestock*" OR “integrated crop-livestock-forestry” OR silvopastoral* OR agropastoral* OR agrosilvopastoral* OR "agroforestry system*") AND (Caatinga OR semiarid OR semi-arid) between the years 2000 and 2023.

Preliminary results: Carbon stock data were extracted from about 53 articles considering the

use of cultivated plants and pasture areas, 28 articles in areas of native Caatinga, and 9 articles in integrated agricultural systems of the Brazilian drylands. In the three types of land use, soil organic carbon stock data were evaluated up to 0.3 meters in depth (Figure 2). Differences in soil carbon stock indicate that integrated agricultural systems have an average of 65 Mg ha-1, followed by native Caatinga with 50 Mg ha-1, and agriculture (including pastures and monoculture) with 27 Mg ha-1. Therefore, the greatest difference observed in soil carbon stock was 38 Mg ha-1 between integrated agricultural systems compared to pasture and monoculture areas. The smallest difference observed in carbon stock was 23 Mg ha-1 between native Caatinga compared to pasture and monoculture areas.

Preliminary conclusions: The adoption of integrated agricultural systems can be considered an opportunity to increase the stock of carbon in the soil. However, several challenges must be considered due to the level of aridity and water availability in the region. In conclusion, the demand for more research to assess the potential of different agricultural systems to store carbon up to one meter deep in the Brazilian semi-arid region is remarkable.

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Abstract Title: Soil Aggregates and Soil Organic Carbon as Quality Indicators in Crop Livestock Forest Integration Systems In The Brazilian Semi-Arid Region

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Abstract: The inadequate uses of the soil and the climatic characteristics have led to the process of environmental degradation, which directly affects the level of productivity in the Brazilian semi-arid region. Therefore, studies that can evaluate the physical quality and structure of the soil to implement of integrated crop-livestock-forest (ICLF) systems are relevant. The aim of this research was to evaluate the impact of adopting different arrangements of ICLF systems in semi-arid Brazil on soil aggregation, and also to assess the potential for using different

aggregation indices as indicators of soil quality. In addition, to evaluate the soil organic carbon content of the different classes of soil aggregates. The study was conducted in an experiment area, located in the Teaching, Research and Extension Unit of the Federal Institute of Science and Technology of Ceará, Campus Limoeiro do Norte. The study was conducted in an experimental area with four ICLF systems: Sorghum, Forage cactus, Massai grass and Buffel grass, each with different spacing between native tree strips (NTS) and native vegetation - Caatinga (NV) with (7m–S7, 14m–S14 and 28m–S28). These systems were compared with an area of native vegetation (NV) and also with NTS. In each treatment five mini trenches (replications) were opened and soil samples were collected at depths of soil of 0-10, 10-20, 20-30 and 30-50 cm. The distribution of water-stable aggregates was evaluated considering the following diameter classes: macroaggregates (diameter>2.00mm), mesoaggregates (2.00-0.25mm) and microaggregates (0.25- 0.05mm), and the weighted mean diameter, geometric mean diameter,aggregate stability index, and sensitivity index were calculated. For the analysis of carbon (C) in the different classes of soil aggregates, the samples were homogenized and the total organic carbon (TOC) levels were determined by the dry combustion method using an elemental analyzer (TOC-Shimadzu, coupled to the SSM-5000A Shimadzu solid sample module). It is observed that at the depth of 0-10cm the NV and NTS presented lower aggregate stability formations in relation to the ICFL systems. On the other hand, in the mesoaggregates, it is observed that at the depths of 10-20cm and 30-50cm, there was greater stability of aggregates in the NV, which will imply a reduction in soil disturbance, which will contribute to the accumulation and decomposition of organic matter. Highlight for the NTS, which showed less stability in the distribution of soil aggregate classes among treatments, with the exception of mesoaggregates at the depth of 20-30cm, which may consider the influence of the cultivation of the ICFL system. Thus, it is concluded that ICFL systems positively influenced the distribution of soil aggregates in the semi-arid.

Keywords: Soil stability; Aggregate index; Land use.

Introduction and Objectives: In Brazil, the semi-arid region continuously covers part of the states of Alagoas, Bahia, Ceará, Paraíba, Pernambuco, Piauí, Rio Grande do Norte, Sergipe, and the north of Minas Gerais, covering a total area of approximately one million km2, representing 12% of the national territory and with approximately 27 million in habitants. This region is still dominated by traditional land use systems (agriculture and pasture), which has led to a combination of factors that have caused environmental degradation in this part of Brazil. However, integrated production systems, such as integrated crop-livestock-forestry (ICLF), have been used as alternative and sustainable ways of improving soil conditions. The adoption of these alternatives has added benefits for soil quality, such as increasing soil carbon sequestration to prevent losses to the atmosphere, which contributes to maintaining soil aggregation and increasing the soil's organic matter content. The soil aggregation is considered the basic unit of soil structure, the formation and stabilization of organic matter, wich significantly affects the storage and turnover of SOC stock. The exchange of carbon (C) in the

soil is the result of natural process an anthropogenic cause, the rate of entry and exit of C in the soil is related to the productivity of vegetation, this balance is disturbed by the change in land use, wich provides a new cycle in agriculture. In Brazil, cultivated and natural pastures occupy approximately 158 ha corresponding to 18.72% of its territory. It is estimated that approximately 20% of the world's pastures are losing productivity due to degradation and inadequate management. In addition to management problems, high temperatures and evapotranspiration, low and irregular rainfall in the region limit the production of plant biomass, which, among other factors, hampers soil organic carbon (SOC) stocks in the semi-arid region. In relation to changes in carbon stocks in pastures, the average stock per hectare is estimated at 6 million (MgC) and 38.663 (MgC.ha) in Brazil. Given the scenario of GHG emissions, management practices in agriculture have been changing in order to mitigate environmental impacts, such as new technologies and management alternatives, like integrated crop-livestock (ICL), crop-forest (ICF), (ICLF) systems and the nature-based solutions (NBS), thus generating economies of scale and production. Studies have shown that the ILPF system achieved a soil carbon sequestration percentage of 7.8% after three years of establishment, representing an increase of 5.5 Mg/ha in the 0-30 cm layer, a value similar to that found in native vegetation. In this context, the aim of this research was to evaluate the impact of adopting different arrangements of integrated ICLF systems in semi-arid Brazil on soil aggregation, soil organic carbon in the different classes and also to assess the potential for using different aggregation indices as indicators of soil quality.

Methodology: The study was carried out in the region of Chapada do Apodi, in the state of Ceará, located in the experimental area at the Teaching, Research and Extension Unit of the Federal Institute of Science and Technology of Ceará (IFCE), Limoeiro do Norte Campus, which has been evaluating different Crop Livestock-Forest Integration (ICLF) systems since 2015, with different spacing arrangements of natural Caatinga trees, with dimensions of 6 × 100 m, positioned in a north-south direction. The experimental area is characterised by predominantly Cambissols. The systems evaluated were: Sorghum (So) with spacings of 7 m (So7), 14 m (So14) and 28 m (So28) between the tree strips, Forage Cactus (Po) with spacings of 7 m (So7), 14 m (Po14) and 28 m (Po28) between the tree strips, Massai grass with spacing of 7 m (Cm7), 14 m (Cm14) and 28 m (Cm28), Buffel grass with spacing of 7 m (Cb7), 14 m (Cb14), 28 m (Cb28) between the tree strips. These systems were compared with an area of native vegetation (NV Caatinga) which was used as a reference for a state of equilibrium, and also with the native tree strips (NTS). For the 7, 14 and 28 m spacings, densities of 1418 (46.15%) trees per hectare were assigned to the 7 m spacing, 925 (30%) to the 14 m spacing and 524 (17.64%) to the 28 m spacing. Soil sampling was carried out in January 2022. Five mini-trenches (replications) were opened in each treatment, and soil samples were collected to a depth of 50 cm in the 0-10, 10-20, 20-30 and 30-50 cm layers. The distribution of wet aggregate stability was assessed considering the following diameter classes: macroaggregates (diameter >2.00 mm), mesoaggregates (2.00 - 0.25 mm) and microaggregates (0.25- 0.053 mm), and the weighted mean diameter (WAD), geometric mean diameter (GMD), aggregate stability index (ASI) and sensitivity index (SI) were calculated. For the analysis of carbon (C) in the different classes of soil aggregates, the samples were homogenized and the total organic

carbon (TOC) levels were determined by the dry combustion method using an elemental analyser (TOC-Shimadzu, coupled to the SSM-5000A Shimadzu solid sample module).

Preliminary results: The aggregate stability analyses for the 28m spacing showed that in the different system treatments ICLF and soil depth there were differences between the layers, which influenced the size and formation of mesoaggregates, resulting in greater quantities of aggregates in relation to the other classes, except in the 0-10 cm depth, which showed greater formation and stability in the macroaggregate class .The microaggregate class had the lowest percentage of aggregates among the treatments and at a depth of 0-50 cm. In the 0-10 cm soil layer, the amount of macroaggregates in Cb28 varied from 34.18% to 23.55% for NV. For the 10-20 cm layer, the distribution of aggregates was greater in the mesoaggregate class, ranging from 39.07% for Cm28 to 29.8% for Cb28. In this layer, the proportion of NV also showed greater stability in the formation of mesoaggregates at 39.02%. For the 20-30 cm layer, the differences were greater, ranging from 44.40% for Cm28 to 35.05% for NV. Cm28 and NTS showed more notable stability in the amount of aggregate formation than NV and the other treatments, while the 30-50 cm layer varied from 48.02% for Po28 to 31.05% for NTS. Considering the average values, in the 0-50 cm depth, the microaggregate class varied from 16.34 % for So28 to 5.51 % for NTS. For the results of the 14 m spacing, it was observed that in all treatments and depths of the ICLF system, the formation of mesoaggregates was significantly higher, and the proportion of macroaggregates in the 20-30 cm layer correspondingly decreased in relation to the other classes. The results observed in the 0-10 cm layer showed greater formation of aggregates in the mesoaggregate class at 47.55% for So14 and 35.07% for NTS, with NV standing out at 39.02% and NTS significantly lower than the other treatments. In the 20-30 cm layer, the treatments ranged from 52.05% for Cb14 to 35.05% for NV, while in the 30-50 cm layer, the treatments ranged from 49.54% for So14 to 31.08% for NTS. NV and NTS stood out as having less stability in the distribution of soil mesoaggregate classes among the treatments, with the exception of macroaggregates at a depth of 0-10 cm, which may be due to the influence of ICFL cultivation. The soil aggregate stability results for MWD and GMD showed higher results in the NTS, So and Cb treatments of the cultivation systems. However, there was a predominance of macroaggregate formation with MWD of 1.45 mm in the So28 treatment, and a lower value in the Cm28 treatment, resulting in 1.27 mm, at depths of 0-10 cm. As such, the MWD represents a good estimate of the class of aggregates most likely to occur in the systems evaluated. The GMD aggregation index showed the highest result of 1.07 cm in the NTS, So28 and Cb28 treatments, and the lowest of 0.80 mm in the Cm28 treatment. When analysing the ASI for each treatment assessed, the NTS treatment showed the highest results with 84.11% and NV was the second highest with 84.02% aggregate stability at the depths.

Preliminary conclusions: The greatest formation of mesoaggregates occurred in all the treatments analysed. Meanwhile, the distribution of water-stable soil aggregate classes showed greater stability in the meso-aggregate class at depths of 20 to 50 cm in the treatments evaluated. In this context, then, the ICLF system is a form of sustainable alternative for the Brazilian semi-

arid region, with the aim of minimizing the constant practices of intensified management and soil disturbance such as harrowing, with the aim of preserving soil structuring, i.e. conserving the formation of aggregates present in the soil. It is therefore possible to state that ICLF systems have had a positive influence on soil aggregation in the semi-arid region analysed, thus maintaining the quality of aggregates close to the condition of native vegetation, favouring the preservation of soil structure. In view of the above, is important to highlight that analyses of soil organic carbon are ongoing.

Diego Silva Siqueira
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Abstract Title: Soil regeneration as a climate strategy and regenerative agriculture

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Abstract: To recovery degraded system an amount of USS 400 billion are spend every year. The use of natural remineralizer is an economic alternative to recovery the quality of soil in degraded areas. The present study took place in the state of Minas Gerais, Brazil and the objective was recovery a degraded pasture applying natural remineralizer in soil. For that soil's sample was collected before and after the application of natural remineralizer in an amount of eight tons per hectare. The results showed that the application of natural remineralizer promoted the formation of new nanoparticles in soil or new types of clay. The application of natural remineralizer also improved the content of organic matter, available phosphorous and cation exchange capacity. The formation of new types of clay helps to maintain the carbon in soil resulting in the reduction of CO2 emissions. The application of natural remineralizer also helps to reduce the emissions from phosphorous fertilizers which impacts in the emissions related to the scope 1; by improving the availability of phosphorous in soil the costs of production is reduced. The use of natural remineralizer is a good and sustainable way to improve soil's quality and help the adoption of sustainable practices by the Brazilian farmers.

Keywords: Soil regeneration, Natural nanoparticles, Bioeconomy, Circular economy.

Introduction and Objectives: Soil should be treated as the most important resource for the maintenance of human kind, because of the ecosystemic function of it. Such function gets us the food that we eat, the clothes that we wear and also the water we drink. Soils also help to

regulate the climate changes by its ability to keep carbon on its structure. Despite these benefits an amount of USS 400 billion are spent every year to improve soil's quality. In Brazil the use of soil natural remineralizer as an alternative input to improve soil's quality is gain force because soil natural remineralizer is a residual of mineral sector and its use can help to reduce the environmental problem of mineral sector and also stimulate the circular economy. Beyond the alternative of using the soil natural remineralizer to improve the soils' function, in tropical soils such as the Brazilian ones we found small particles that influence the natural ability of soil to exercise its functions. However, the presence of these nanoparticles is related to the type of rock the soil come from. The use of natural remineralizer can help in the formation of new nanoparticles in soil which help in regenerate degraded area. There are also other areas of research using synthetic nanoparticles to recovery degraded areas which complement the use of natural remineralizer. In this context, the objective of this research was verifying the influence of natural remineralizer in the improvement of soil's attributes such as organic matter content, available phosphorous, cation exchange capacity and soil magnetism which is related to the presence of soil's nanoparticles.

Methodology: The experimental area was a degraded pasture located in the state of Minas Gerais. The soil of the area came from the sandstone rock. An amount of eight tons per hectare of soil natural remineralizer was applied to recover the pasture and to verified if the amount promoted changes in the chemical attributes of the soil. The soil natural remineralizer showed 0,30 mm of grain size and mineralogical composition of FeO3, Al2O3,SiO2 and TiO2. The soil's samples were collected before and after the application of the soil natural remineralizer to determine the magnetism of the soils, the content of organic matter, phosphorus and cations exchange capacity (CTC). The samples happened in different times to verify the influence of soil natural remineralizer on the behaviour of soil attributes. After soil's collection the samples were analysed to determine the content of organic matter, phosphorus and CTC and soil's magnetism before and after the application of soil natural remineralizer.

Preliminary results: The application of natural remineralizer in soil promoted a formation of new nanoparticles or new types of clay in soil because the values of soil magnetism without soil natural remineralizer was 0,20 and after the application the value was 0,35 an increase of 75% on the index of soil magnetism. The presence of these new type of clay also promoted the improve of the soil quality, because we observed an increase of 49% in the content of organic matter. We also noticed that the availability of phosphorus increased 187,5% with the application of the soil natural remineralizer in the soil. The CTC of the soil also increased 55,18% after the application of soil natural remineralizer. It is important to highlight that the presence of these new type of clay promote a protection of the carbon in soil and hence helping the mitigation of CO2 emissions.

Preliminary conclusions: The soil natural remineralizer showed a great potential to improve soil's quality and an alternative of input to improve the amount of phosphorus in soil and reduce the dependence of Brazilian agriculture in external inputs. The improvement of phosphorus

availability caused by the use of remineralizer in soil contributes to the reduction of its use, reduction of the production's costs and also the reduction on emissions caused by the phosphorus fertilizers related in the scope 1 in the GHG inventory. The formation of new nanoparticles in soil because of the application of soil natural remineralizer promoted an increase of the specific surface area which reflected in the development of CTC and organic matter in soil. Beyond an alternative of reuse the residual material produced by the mineral sector which can cause a serious environmental problem.

Geraldo Lavigne de Lemos
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Abstract Title: Brazilian regulation on Nature-Based Solutions: relevance, references and gaps

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Abstract: The theme of nature-based solutions has emerged as a promising alternative for tackling socio environmental challenges. It is an approach that seeks to use nature as a source of solutions to problems that affect people's quality of life and the planet's sustainability in the context of climate change. Nature-based solutions can be applied in different areas, such as water resource management, urban planning, and sustainable agriculture, among others. Implementing these solutions can bring significant benefits in terms of conserving ecosystems, reducing the risk of natural disasters, adapting
to climate change and promoting local communities' social and economic well-being. In this sense, it is crucial to understand the rules, laws and public policies related to the issue. This study seeks to explore the current relevance of the issue and its impact on society, understand the main rules on the subject in Brazil and other countries, and propose solutions for the identified regulatory gaps. The study adopted a bibliographical and exploratory analysis methodology. The data found points to the existence of rules on nature-based solutions in several countries, while in Brazil, the issue is dealt with in a generic and sparse manner. In any case, in Brazil and other countries, standards on nature-based solutions are incipient and, in most cases, require further regulation. Significant gaps were identified on the subject, but much content is noted in international legislation that could serve as a basis for future regulation of the subject in Brazil. From the experiences found, it is possible to extract contributions for more assertive regulation in national normative proposals.

Keywords: nature-based solutions; Brazilian regulation; regulatory gaps.

Introduction and Objectives: According to Fraga (2021), nature-based solutions (NBS) are

increasingly being used worldwide to tackle various environmental, social and economic challenges. It is an approach that seeks to use nature as an ally to solve problems arising from climate change rather than seeing it as a mere source of resources to be exploited. In this sense, using NBS can bring benefits such as improving the quality of life of communities, protecting biodiversity, adapting to climate change and mitigating its effects. This research shows that several countries have legislation and projects underway aimed at NBS, such as Costa Rica, Australia and New Zealand. In Brazil, there are still few specific rules on the subject. However, it is worth noting that there are examples of projects underway in some states and municipalities and environmental rules that apply to NBS at all levels - federal, state and municipal. In this context, it is of fundamental importance to understand how NBS are dealt with in Brazil and to benchmark this issue in other countries in order to be able to comment on how NBS can be developed.

Methodology: The research adopted a bibliographic and exploratory approach to investigate Brazilian regulation of nature-based solutions. The bibliographical approach allowed for an in-depth analysis of the existing literature on the subject. In contrast, the exploratory approach provided the opportunity to identify new insights and generate hypotheses for future research, such as a bill on the subject. The research problem addressed in this study is Brazilian regulation on the subject. This problem is of great relevance to the field of study, as regulation of nature-based solutions would be paramount for Brazil's political, legal and environmental development. For the bibliographical research, various data sources were used, including books, scientific articles, reports, official documents and relevant publications in the field. Data sources were selected based on their relevance and quality, ensuring that reliable and up-to-date information was obtained for the analysis, mainly by comparing with international standards/projects on the subject. The process of collecting bibliographic data involved a systematic search of academic databases, digital libraries and other relevant sources. Keywords and inclusion and exclusion criteria were used to ensure the selection of literature pertinent to the research topic. The data collected was organized to facilitate analysis and the identification of patterns and trends. It is essential to recognize the inherent limitations of bibliographical and exploratory research. Among other limitations are the limited availability of relevant literature on the subject and the impossibility of generalizing the results to contexts other than the country of origin. These limitations must be considered when interpreting this study's findings.

Preliminary results: There is some international legislation that we can use as inspiration, such as the United Nations General Assembly Resolution A/RES/72/277, which includes explicit references to nature-based solutions. The resolution encourages governments and other stakeholders to promote the integration of nature-based solutions into policies, strategies and

action plans related to sustainability and climate change. In addition, the European Union recently adopted the EU Biodiversity Strategy for 2030, which includes a specific objective of restoring degraded ecosystems, protecting and enhancing valuable ecosystems, and increasing the use of nature-based solutions. The strategy outlines a roadmap for integrating nature-based

solutions into policies and investments across the EU. In addition, some countries such as Costa Rica, Colombia and Mexico, like Brazil, have a rich biodiversity and are known for implementing public policies and programs that promote nature-based solutions in their conservation strategies. These countries share many of the same challenges Brazil faces, including the degradation of natural ecosystems, the loss of biodiversity and the need to balance economic development with environmental conservation. Costa Rica is one of the leading countries in nature-based solutions and has several initiatives and laws that promote the restoration and conservation of ecosystems and the use of nature-based solutions to tackle environmental and social challenges. One of the main laws dealing with nature-based solutions in Costa Rica is the Payment for Environmental Services Law (Law No. 7575/1996), which establishes a system of financial incentives for landowners who preserve forests and other natural ecosystems and those who restore them. This system is considered a successful example of how nature-based solutions can promote the conservation of biodiversity and the protection of water resources. In addition, Costa Rica recently adopted the National Strategy for Nature-Based Solutions (2020-2030), which establishes an action plan to increase the use of nature-based solutions in various sectors, including agriculture, energy, infrastructure and tourism. The strategy also aims to increase the country's resilience to climate change and reduce poverty through nature-based solutions. Another relevant piece of legislation in Costa Rica is the Biodiversity Law (Law No. 7788/1998), which establishes the National System of Conservation Areas and the government's obligation to protect biodiversity and promote the sustainable use of natural resources, including nature-based solutions. Therefore, It is possible to look at these countries as references and draw inspiration from their public policies and conservation programs to implement nature-based solutions in Brazil. Similarly, the experiences of other countries can help define more assertive cases based on successful examples that can be repeated, avoiding failures.

Preliminary conclusions: From the literature reviewed, it is possible to conclude that nature-based solutions have been gaining increasing attention worldwide as an alternative for tackling environmental and social challenges. Several countries have created legislation and policies to encourage the use of nature-based solutions, seeking to guarantee the protection and conservation of biodiversity and ecosystem services while delivering social benefits and conditions for adapting to climate change. In Brazil, there are some ongoing NBS initiatives, such as the River Planters Project and the Water Producer Program, which aim to recover degraded areas and conserve water resources. However, much must be done to ensure that nature-based solutions will be widely disseminated and used in the country. The literature consulted highlights the importance of an integrated and participatory approach to developing nature-based solutions, involving various sectors of society and valuing traditional and local knowledge. In addition, it is essential to create incentives and funding mechanisms to promote

the implementation of nature-based solutions on a large scale. According to all the research presented here, the challenges faced in implementing NBS in Brazil include the lack of awareness and technical training among the population and public managers and the need for a

regulatory framework to encourage and guide the implementation of these solutions. Because of this, the subject of NBS must be widely discussed and disseminated in Brazil, seeking to foster initiatives that can contribute to their implementation and dissemination in different regions of the country. Using nature-based solutions is an essential strategy for conserving biodiversity and ecosystem services, as well as for sustainable development and improving the quality of life of local populations. Governments, civil society and the private sector must work together to create favourable conditions for the implementation of these solutions around the world.

Giovanna Pereira Correia
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Abstract Title: Nanotechnology for hydroponic applications: Development of Metal-organic frameworks (MOFs) for nutrients releasing.

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Abstract: The development of efficient crop fertilizer technologies has become increasingly important; however, their high cost, complex production processes, and potential environmental risks have limited their application. In this regard, the design of new materials with highly organized structures that contribute to controlled nutrient release is necessary. Thus, the present study focuses on a class of materials known as MOFs, with their crystalline structure optimized through the formation of a 3D porous network acting as a host for nutrient-rich components for agricultural applications. The dataset reveals that the enrichment effect of Fe-Phosphate-amino-based MOF in nutrient solutions can be adopted as a strategy to improve growth parameters and the quality of hydroponically grown crops.

Keywords: Hydroponic, Cultivation, Nanotechnology, Metal-Organic framework, Controlled nutrient release.

Introduction and Objectives: Hydroponics is an innovative plant cultivation technique that eliminates the use of soil as a substrate, and it is increasingly being applied in enclosed environments such as greenhouses, hothouses, and even indoor systems like vertical farming in urban buildings. In this system, plant roots are immersed in a nutrient solution containing all essential nutrients for healthy growth, allowing plants to develop efficiently and sustainably. One of the main benefits of hydroponics is significant water savings compared to conventional agriculture. While in traditional agriculture, a significant portion of water is lost through leaching and evaporation, in hydroponic systems, water is recirculated, significantly reducing

water consumption. To ensure healthy plant growth, it is essential to provide an adequate supply of nutrients that plays crucial roles in plant physiological functions, and their deficiency can result in slow growth. In hydroponics, nutrients are divided into two main categories: macronutrients and micronutrients, in which macronutrients are required in relatively large quantities and includes nitrogen (N), phosphorus (P), potassium (K), calcium (Ca), magnesium (Mg) and sulfur (S), and micronutrients, required in smaller quantities, but are also vital. They include elements such as iron (Fe), zinc (Zn), manganese (Mn), copper (Cu), boron (B), molybdenum (Mo), and chlorine (Cl). Controlled nutrient release is a crucial aspect of hydroponic cultivation. Ensuring that nutrients are delivered gradually to plants over time is essential for efficient absorption and the prevention of resource wastage. Various advanced materials, such as nanoparticles and microparticles, have been studied and applied to optimize controlled nutrient release in hydroponic systems. These materials can be used to encapsulate nutrients, allowing them to be released gradually as the nutrient solution comes into contact. Nanotechnology has played a significant role in the search for innovative solutions for controlled nutrient release in hydroponics and the application of nanomaterials, such as Metal Organic Frameworks (MOFs), has been explored for this purpose. Metal-organic frameworks (MOFs) are hybrid metal-organic materials with adjustable pore sizes and symmetrical ordering through the self-assembly of metal ions or clusters with organic ligands. MOFs possess intrinsic physical and chemical properties that can be controlled through parameters such as specific surface area, pore size, and material stability, making them suitable for a variety of applications. Control over pores makes these materials promising for the controlled delivery of essential nutrients for socio-environmental development. Additionally, MOFs can be sustainably synthesized using biomolecules or biomass-derived molecules as ligands, making them biocompatible and biodegradable materials, which are highly desirable for agricultural applications.

Methodology: The material proposed in this study was obtained through a hydrothermal method using water as a solvent. The physicochemical properties were analysed using techniques such as Raman spectroscopy, FT-IR, and UV-Vis reflectance in the solid state. Other techniques, such as thermogravimetry (TGA), were employed to analyse the material's thermal decomposition. The crystalline and molecular structure of Fe(III) MOF was determined by single-crystal and powder X-ray diffraction. The resolution of the crystalline structure provides a better understanding for material optimization, especially for the use of its properties related to surface area and porosity.

The release of nutrient components (Fe, P, and N) and the degradation of the material in hydroponic medium were studied using inductively coupled plasma optical emission spectrometry (ICP-OES) with pH control.

Preliminary results: The nutrient release behaviour in water during the slow and prolonged degradation of MOF confirms its potential for application not only in hydroponic systems but also for enriching the nutrient matrix in soil.

Preliminary conclusions: The use of MOFs for controlled nutrient release in hydroponics can bring various benefits. Firstly, it improves the efficiency of fertilizer use, reducing nutrient loss through leaching and, consequently, reducing the negative environmental impact associated with excessive fertilizer use in traditional agriculture. Thus, the use of these advanced materials allows better control over nutrient availability to plants, ensuring more adequate and personalized nutrition according to the specific demands of each crop.

Henrique Medeiros Vignati
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Abstract Title: Two worlds, One Goal: A comparative Analysis of Nature-Based Solutions (NBS) from the Oil Sector and the Global perspective

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Abstract: Nature-based Solutions (NbS), which emerged in the late 2000s, can be understood as a set of alternatives that were inspired, copied, or based on natural processes to generate social, environmental, and economic benefits for society (Fraga & Sayago, 2020). They can potentially protect, sustainably manage, and restore natural and modified ecosystems, and also address social challenges in an effective and adaptive way to promote social well-being and benefits to biodiversity (Cohen-Shacham et al. 2016). To a larger extent, the NbS concept was developed in a capitalist Western economies context and thus inherently incorporates values, viewpoints, power, and political dynamics. Intrinsic problems in this context such as colonialism and power imbalance globally affect access to resources and patterns of spatial development relevant to NbS. On the other hand, Nature stands as a possibility of response to present problems, considering that NbS encompasses a wide range of ecosystem-related approaches (Cohen-Shacham et al., 2016; Nesshover et al., 2017; Irfanullah, 2021). Therefore, we can convey this idea as a solution for capital and services, reinforcing nature as an opportunity that can help us to achieve positive outcomes for society's problems (White et al. 2021; Nesshover et al. 2017; Shacham et al., 2016). Moreover, we can relate NbS's integration opportunities to environmental goals, public policy sectors, businesses, and other practices that have not yet considered the value of Nature as an ally for sustainable decision-making (Nesshover et al. 2017). The purpose of this paper is to understand, through a critical review of the literature, the global view on the practices of NbS and compare it to the traditional oil sector

perspective. Arguably, the oil sector could benefit from this approach, since it has long

contributed to environmental issues over decades. Thus, oil companies are important stakeholders to consider in the process of decarbonizing the global economy, which was proposed in the Paris Agreement (2015). Considering that social issues are affected by, and have an effect on diverse stakeholder groups, it is important to involve these groups in the problem-solving process and thoroughly understand their perspective to reach an optimized solution (Nesshover et al., 2017).

Keywords: Oil, Nature-based Solutions, Sustainable development.

Introduction and Objectives: Anthropogenic activities have undeniably left a remarkable footprint on Earth, mostly related to large scale fossil fuel consumption, which arguably contributed to, for example, ocean acidification, deforestation, and species extinction. (Lucon, 2022). According to the Sixth Assessment Report from the Intergovernmental Panel for Climate Change (2021), Human activities, principally linked to greenhouse gas emissions, have unequivocally caused global warming. In this sense, global greenhouse gas emissions have continued to increase toward unprecedented levels arising from unsustainable energy use. In 2019, atmospheric CO2 concentration achieved the highest historical value of 410 ppm over 2 million years (IPCC, 2023). That brings a necessity to think of solutions based on the core polluters, evaluating what sector can be the principal in decarbonization.

The early postwar era witnessed a series of shocks in oil markets mostly due to regional conflicts that unfolded with global effects (Hamilton, 2010). As a consequence, comes the emergence of an environmentalism approach alongside discussions on peak oil, which resonated among the decision-making stakeholders. Conversely, in the 1970s, when price increases in oil were taking part in the inflationary pressures (Hamilton, 2010), the Club of Rome came up with a strategic ideology to maintain the USA's hegemony. With a counter offensive for the propagation of the idea of zero growth, neo malthusianism, and environmental approaches, the US's strategy targeted mainly Europe and Japan (Amin, 1977). Also attributed to the Club of Rome, the sustainable development concept and the report on limits to development arose. The organization of the Stockholm Conference, in 1972, was mainly articulated by Maurice Strong, who became the first executive director of the United Nations Environment Programme (UNEP) but also happened to be an oil tycoon (Camely, 2018). Arguably, these contradicting viewpoints still remain on the same side of the table: sometimes advocating for a low-carbon economy, while relying on perpetuating a carbon-intensive activity. However, solutions pass by decarbonization and NbS, since NbS can be understood as a set of alternatives that were inspired or based on natural processes to generate social, environmental, and economic benefits for society (Fraga & Sayago, 2020). There are still uncertainties and gaps, in terms of overlap and delineation around associated concepts such as stakeholder participation, making it difficult to consider the imprecision and uncertainties of the concept itself (Nesshover et al., 2017). In conclusion, this study aims to answer the question:

what is, both, the worldwide view and the oil sector view on decarbonization? The objective is to compare the viewpoint of the oil industry about NBS along with the worldwide view on the theme to obtain a conclusion about what guides each of the perspectives on decarbonization and NBS.

Methodology: The critical review of the literature intended in this study composes the following criteria, used to select the most relevant articles worldwide to use in this paper. The selected articles were based on scientific databases (Scopus, Clarivate, and Google Scholar) using appropriate keywords, based on the theme. It was selected sustainability reports from oil companies, in order to know some about how they inform about NbS and Decarbonization and relevant authors in the intended theoretical frame (eco marxist/marxist) such as John Bellamy Foster, Enrique Leff, Antonio Carlos Diegues, and more. The main goal is to select references that provide a foundation for comprehension, understanding, and analysis of the proposed theme in a socio-historical process for the establishment of the actual climate agenda. To achieve this objective, a brief literature review regarding sustainability, fossil fuels, sustainable development, climate change, decarbonization, Nature-based Solutions, ecological imperialism, strategy for the oil sector and geopolitics of energy will be conducted.

Preliminary results: It is expected that, with this article, it is possible to contribute to the general notion of the NbS in Brazil, and to further understand its applicability, both, for the oil sector and decarbonization. It is conjectured that this contribution helps the development of the NbS theme, in terms of promoting climate change adaptation and decarbonization. Mainly in the Global South, affected by the imposition of imperial Western ideologies, that restrain integration within the traditional population and their knowledge, affecting the applicability of NbS in Latin America, for example. Given these points, assuring a possibility for them to contribute to the solutions also can make that it comes Nature-based.

Preliminary conclusions: Currently, the view on decarbonization worldwide is that we need it to solve environmental problems, such as climate change. It is known that anthropogenic climate change is an unquestionable fact (IPCC, 2023), given this, and the actual scenario of oil development it is important to enlarge the application of solutions that come from nature, and go towards nature. That is were we can fit NbS, but it is crucial that this decision don't overtake traditional knowledge and include these cosmologies and epistemologies, given that it can potentially surpass them and end in "welfare" politics, that potentially ignore traditional knowledge and maintain the historic imperial domination over south countries.

José Igor Almeida Castro
ESALQ/ USP

Abstract Title: Effects of Improved Pastures and Integrated Systems on Soil Carbon Sequestration in Brazil

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Abstract: Brazil offers outstanding opportunities for contributing to climate change mitigation through carbon sequestration in pasture systems. Although several studies have been published assessing soil organic carbon (SOC), there is still a lack of information on the potential for carbon sequestration by improving pasture management, especially when integrated production systems are implemented. We aimed to derive factors for SOC stock change and potential sequestration rates for the conversion of extensive pastures into improved management and integrated production systems of crop-livestock-forest (CLFS), crop-livestock (CLS), and livestock-forest (LFS). We gathered primary studies by a systematic review process to build a database for Brazilian pasturelands, then, a mixed-effect linear regression model was fitted to estimate carbon management factors coefficients and SOC stock change rates. We included 283 data pairs comparing a reference (extensive or degraded pasture) and treatment, distributed in 37 field experiments from 30 published papers. The results pointed out that for 20 years, at a 0-30 cm depth, the improvement of exclusively pasture systems has the potential to increase SOC stocks by 18% from extensive pastures, while the adoption of integrated production systems can enhance by 34%, for LFS, 28%, for CLFS, and 3%, for CLS. We used these management factors to analyze the C stock change rates, providing a potential to sequester over a period of 20 years, in 0-30 cm depth, 0.21 Mg C ha $^{-1}$ year^{-1}, for improved pastures, 0.39 Mg C ha $^{-1}$ year^{-1}, for LFS, 0.03 Mg C ha $^{-1}$ year^{-1}, for CLS, and 0.34 Mg C ha $^{-1}$ year^{-1}, for CLFS. The LFS presented the best opportunities to store C in soil, thus, we suggest more long-term research on this system to understand how time affects the change rates. These C factors contribute directly to national greenhouse gas emission inventories updates since they typically develop estimates based on regional studies. The results also raise new opportunities to assess the carbon change dynamics for specific categories of integrated production systems.

Keywords: Crop-livestock-forestry; Soc change; Mixed-effect regression model.

Introduction and Objectives: Brazil offers outstanding opportunities for contributing to climate change mitigation through carbon sequestration in pasture systems. Although several

studies have been published assessing soil organic carbon (SOC), there is still a lack of information on the potential for carbon sequestration by improving pasture management, especially when integrated production systems are implemented. We aimed to derive factors for SOC stock change and potential sequestration rates for the conversion of extensive pastures into improved management and integrated production systems of crop-livestock-forest (CLFS), crop-livestock (CLS), and livestock-forest (LFS).

Methodology: We gathered primary studies by a systematic review process to build a database for Brazilian pasturelands, then, a mixed-effect linear regression model was fitted to estimate carbon management factors coefficients and SOC stock change rates. We included 283 data pairs comparing a reference (extensive or degraded pasture) and treatment, distributed in 37 field experiments from 30 published papers.

Preliminary results: The results pointed out that for 20 years, at a 0-30 cm depth, the improvement of exclusively pasture systems has the potential to increase SOC stocks by 18% from extensive pastures, while the adoption of integrated production systems can enhance by 34%, for LFS, 28%, for CLFS, and 3%, for CLS. We used these management factors to analyze the C stock change rates, providing a potential to sequester over a period of 20 years, in 0-30 cm depth, 0.21 Mg C ha $^{-1}$ year^{-1}, for improved pastures, 0.39 Mg C ha $^{-1}$ year^{-1}, for LFS, 0.03 Mg C ha $^{-1}$ year^{-1}, for CLS, and 0.34 Mg C ha $^{-1}$ year^{-1}, for CLFS.

Preliminary conclusions: The LFS presented the best opportunities to store C in soil, thus, we suggest more long-term research on this system to understand how time affects the change rates. These C factors contribute directly to national greenhouse gas emission inventories updates since they typically develop estimates based on regional studies. The results also raise new opportunities to assess the carbon change dynamics for specific categories of integrated production systems.

Laudelino Vieira Da Mota Neto
Sao Paulo State University Unesp

Abstract Title: Soil Aggregates and Carbon Cycling in Maize-Forage Intercropped Systems Fertilized with Nitrogen

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Valadares Galdos, Soil Carbon Specialist, Rothamsted Research, Harpenden, UK. Ciro Antonio Rosolem, Professor, Crop Science Department, FCA, São Paulo State University – UNESP.

Abstract: Intercropping maize with forages is an alternative for intensifying food production while building up soil resilience strategies on a changing climate. Our research aimed to investigate to what extend the new carbon (C) input affects the cycling of the already stabilized soil C, soil organic matter (SOM) fractions and within micro (<0.250mm) and macroaggregates (>0.250mm), especially when fertilized with nitrogen (N) in a seven-year experiment with maize intercropped with ruzigrass, palisade and Guinea grass fertilized or not with N. The absence of N resulted in larger aggregates compared with N fertilization. Intercropping increased δ13C values in the bulk soil (8.9%), in particulate (4.4%) and mineral-associated (7%) organic matter fractions, and within micro and macroaggregates (7.5%) through the soil profile (0-40cm) disregard forage species and N application. However, N supply increased the intercropping-carbon derived in the particulate organic matter 6.3% at the 10-20 cm soil depth. Guinea grass resulted in 10.5% more carbon into aggregates compared with ruzigrass. Yet, aggregates larger than 2.0 mm showed on average 36% more carbon than that beheld at 0.105 mm aggregates across the soil profile. Soil total N was not affected across >2.0, 1.0, and 0.5-mm aggregates, but was 23.9% higher than that at the smallest aggregate. These findings contribute to a better understanding of C dynamics in intercropped systems. Our results showed that N supply resulted in smaller soil aggregates compared with no N, but the mechanisms are unknown and needs further scrutiny. Intercropping replaces the already stabilized carbon in different soil structures and carbon pools, but there are no consistent differences between forage species and response to nitrogen rates. São Paulo State Research Foundation (FAPESP), grant - 2021/05167-7. AGRISUS, grant - 2918/20.

Keywords: intercropping; carbon dynamics; soil physics.

Introduction and Objectives: Intercropping maize with forages is an alternative for intensifying food production while building up soil resilience strategies on a changing climate. Our research aimed to investigate to what extend the new carbon (C) input affects the cycling of the already stabilized soil C, soil organic matter (SOM) fractions and within micro (<0.250mm) and macroaggregates (>0.250mm), especially when fertilized with nitrogen (N) in a seven-year experiment with maize intercropped with ruzigrass, palisade and Guinea grass fertilized or not with N.

Hypothesis

H1: the input of below and aboveground biomass, especially under nitrogen supply, would lead to higher aggregation and carbon content into macroaggregates.

H2:Palisade grass can increase the formation of larger macro aggregates compared to the other grasses.

H3:the grasses would increase the C input into the soil, which could be traced by the reduction in δ13C values in the bulk soil samples, in the SOM fractions and within macro and

microaggregates after seven years.

H4:the effect of grasses on the parameters evaluated could reach the whole soil profile (0-40 cm) with a more consistent effect of the forage grasses and nitrogen levels at the topsoil layer(0-10cm).

Methodology: monoliths were collected in September 2021 from a seven-year experiment at the 0-10, 10-20 and 20-40 cm. The monoliths were manually dismantled breaking them into smaller aggregates. The samples were dried at room temperature and screened using a set of sieves of 8 and 4 mm. The aggregates remaining on the 4 mm screen were separated for aggregate stability analysis. Bulk soil samples were collected as a composite of three cores at 0-10; 10-20 and 20-40 cm depths.

Analysis of aggregates

Briefly, we used a method adapted for tropical soils (SILVA; MIELNICZUK, 1998), which uses a vertical oscillation system based on wet sieving separation of aggregates into a set of sieves - 2.0, 1.0, 0.5, 0.25 and 0.105 mm. The aggregates remaining over each sieve were transferred to plastic cups with lids, dried in an air-forced oven (60 ºC) and weighed. The mean weight diameter (MWD), geometric mean diameter (GMD), and the water-stable aggregates stability rate (WSAS) were assessed using the equations as proposed by (ZHOU et al., 2020). The portion of aggregates recovered on the sieve >2mm was presented as percentage (%) relative to the 45g of the soil sample used for analysis.

Physical soil organic matter fractionation

The SOM physical fractionation was adapted from CAMBARDELLA; ELLIOTT (1993). Briefly, 5 g of soil were weighed in 200-mL plastic cups with lids followed by 20 mL of a sodium hexametaphosphate solution, and then shook for 15h. The sample was screened over a 0.053-mm (53 µm) sieve, rinsed with tap water until phase out clay. The POM fraction > 0.053-mm was dried out in an oven at 50°C. The fraction < 0.053-mm deemed mineral-associated organic matter (MAOM) was recovered and dried at 50°C.

Total carbon and nitrogen measurements

Subsamples taken from bulk soil samples, POM, MAOM and aggregates recovered at 2, 1, 0.5, 0.25 and 0.105 mm sieves were air-dried and ground to a finer texture using a ball-mill after shaking for 45s, and total carbon (TC) and nitrogen (TN) content were measured using a CHN-2000 analyzer (Leco Corp., St. Joseph, MI, USA).

13C natural abundance measurement

The natural 13C isotope abundance were measured in the bulk soil, POM and MAOM fractions. The aggregates were separated into macro (> 0.25 mm) and microaggregates (< 0.25 mm). A sample of 10- 20.000 µm was placed in a tin capsule. The analyses were performed using an isotopic mass spectrometry (CF-IRMS; Delta 187 V, Thermo Scientific, Germany) equipped with a continuous flow ratio coupled with an elemental analyzer (Flash HT, Thermo 188

Scientific, Germany) using a gas interface (ConFlo IV, Thermo Scientific, Germany). The values were expressed as the relative difference of isotopic ratio (δ13C - R(13C/12C)), in parts per thousand (‰). The Vienna PeeDee Belemnite (V-PDB) was the standard sample (COPLEN, 2011). The uncertainty was estimated in ±0.15 ‰ (n=10), and the results were normalized using the NBS-22 certified reference standard.

Preliminary results: The absence of N resulted in larger aggregates compared with N fertilization. Intercropping increased δ13C values in the bulk soil (8.9%), in particulate (4.4%) and mineral-associated (7%) organic matter fractions, and within micro and macroaggregates (7.5%) through the soil profile (0-40cm) disregard forage species and N application. However, N supply increased the intercropping-carbon derived in the particulate organic matter 6.3% at the 10-20 cm soil depth. Guinea grass resulted in 10.5% more carbon into aggregates compared with ruzigrass. Yet, aggregates larger than 2.0 mm showed on average 36% more carbon than that beheld at 0.105 mm aggregates across the soil profile. Soil total N was not affected across >2.0, 1.0, and 0.5-mm aggregates, but was 23.9% higher than that at the smallest aggregate.

Preliminary conclusions: Our results unveil to what extend intercropping maize with forage species supplied or not with N affects soil aggregation, C cycling and SOM fractions within macro and microaggregates in a seven-year experiment and contribute to a thorough understanding of C dynamics in intercropped systems. Our results showed that N supply resulted in smaller soil aggregates compared with no N, but the mechanisms are unknown and needs further scrutiny. Intercropping replaces the already stabilized carbon in different soil structures and carbon pools, but there are no consistent differences between forage species and response to nitrogen rates.

Daniel Aquino De Borba
University of São Paulo

Abstract Title: Impact of Converting Pasture Areas into Sustainable Agriculture on Soil Organic Matter Dynamics

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Abstract: Soil carbon sequestration is one of the main strategies for reducing the growing CO2 emissions caused by human activities in recent decades. In order to meet the world demand for food, fiber and biofuels, agricultural areas cultivated in Brazil have expanded strongly in the last decade. The change in land use and the intensification of production systems alter the concentration of CO2 in the atmosphere, transforming the soil into a sink or emitter of carbon (C), influencing climate change. In this sense, the replacement of areas of natural vegetation by areas of pasture or agricultural crops has been associated with the absence of conservationist management practices, recent publications have shown that sustainable management practices contribute to the increase of soil C levels, restoration of soil health and GHG mitigation. Our project aims to evaluate the impact of converting pasture areas (PA) to sustainable agriculture (AS) on soil organic matter (SOM) dynamics, covering tropical and
subtropical climates. Through quantification of soil C and N contents under the effects of land use change, physical fractionation of total soil OM, through techniques that differ in terms of aggregation, composition, permanence and function (e.g. MOAP and MOP) , which will allow with greater sensitivity to identify changes in SOM under different uses and managements and durations, and to understand the dynamics of SOM. In the end, the data will be integrated to evaluate the effects on the conversion of PA into AS, and the different levels of intensification of the productive systems. In this way, we will quantify the impacts generated on SOM, C stocks and stabilization and permanence in the
soil, through this, allowing the identification of management practices with the potential to mitigate C in the tropics and subtropics of Brazil, thus guaranteeing a sustainable development of agriculture.

Keywords: Conservation practices; organic carbon stock; soil management; quality and quantity of soil organic matter.

Introduction and Objectives: Soil is fundamental for the regulation of gaseous exchange in the atmosphere, in particular, the mitigation of carbon dioxide (CO2), one of the main greenhouse gases. The change in land use and intensification of production systems can promote the loss of carbon (C) from the soil. The use of conservation management practices contributes to the increase in soil C levels and is essential for the development of sustainable agriculture.Our project aims to evaluate the impact of converting pasture areas (PA) to sustainable agriculture (AS) on soil organic matter (SOM) dynamics, covering tropical and subtropical climates. To quantify the impacts generated on SOM, C stocks and stabilization and permanence in the soil, through this, allowing the identification of management practices with the potential to mitigate C in the tropics and subtropics of Brazil, thus guaranteeing a sustainable development of agriculture.

Methodology: The soil will be sampled at nine points for each use up to a depth of 1 meter. To quantify the C and N contents of the soil under the effects of land use change, the elemental analyzer will be used in the quantitative aspects of SOM. In addition, the physical fractionation of total soil OM, using techniques that differ by aggregation, composition, permanence and function (e.g. MOAP and MOP), which will allow, with greater sensitivity, to identify changes

in SOM under different uses and managements and durations, and understand the dynamics of SOM. Microbiological changes will be evaluated by means of β-glicosidase activity, C and N determination of microbial biomass and soil DNA extraction. Likewise, for qualitative analysis of soil biochemical changes, laser-induced fluorescence spectroscopy (FIL) analysis will be performed to identify the degree of SOM wetting. At the end, the data will be integrated to evaluate the effects on the conversion of PA into AR, and the different levels of intensification of the productive systems.

Preliminary results: In the end, the data will be integrated to evaluate the effects on the conversion of PA into AS, and the different levels of intensification of the productive systems.

Preliminary conclusions: In this way, we will quantify the impacts generated on SOM, C stocks and stabilization and permanence in the soil, through this, allowing the identification of management practices with the potential to mitigate C in the tropics and subtropics of Brazil, thus guaranteeing
a sustainable development of agriculture.

Letícia Oliveira Bispo Cardoso
University of São Paulo

Abstract Title: Comparison of microalgal and cyanobacterial hydrolysate for 3G bioethanol production

Authors' Names & Affiliation Institutions of all authors (in order for publication): Letícia Oliveira Bispo Cardoso, Dielle Pierotti Procopio, Bruna Bacaro Borrego, Louise Hase Gracioso, Cassius Vinicius Stevani, Renato Sanches Freire, Claudio Augusto Oller do Nascimento, Elen Aquino Perpetuo.

Abstract: Brazil, the second-largest ethanol producer globally, faces challenges related to edible sources (1G) and lignocellulosic material (2G), paving the way to 3G bioethanol, which is derived from the hydrolysate photosynthetic microorganisms' biomass, that can thrive without arable land or potable water, relying solely on light, CO2, and nutrients. This project assessed the viability of using distinct photosynthetic microorganisms as feedstock for 3G

ethanol production, i.e., a microalgal (Didymogenes sp.) and cyanobacterium (Synechocystis sp.) strains. Cultivation involved triplicate static growth in Erlenmeyer flasks with BG-11 medium, constant CO2 atmospheric bubbling at 100 µmol photons m-2 s-1 and 21 ± 3ºC. The cellular growth was measured by optical density at 750 nm, and gravimetry post-lyophilization. Dilute acid hydrolysis [1% (v/v) H2SO4, autoclaving at 121ºC for 30 minutes] was performed on the final biomass, followed by neutralization. Metabolites quantification generated after acid hydrolysis (organic acids, furanic compounds, and glucose) and after fermentation (ethanol) were carried out using HPLC. The fermentation was performed in duplicate using the cyanobacterial hydrolysate (CH), the microalgal hydrolysate (MH), and YPD medium for comparison, set to 10 g L-1 of glucose. The flasks were kept at 30ºC and 150 rpm for 24 hours. So far, the results obtained showed that under the same cultivation conditions, Didymogenes sp. presented biomass productivity of 0.11 ± 0.01 g/L.day-1 similar to 0.12 ± 0.01 g/L.day-1 obtained by Synechocystis sp. over 11 days of cellular growth with 7 days of carbohydrate accumulation. The glucose production was significantly higher in the cyanobacterial strain, reaching 37.78 ± 0.20% (w w-1) in comparison to 15.43 ± 1.26% (w w-1) obtained by the microalgae. The dilute acid hydrolysis used to obtain the hydrolysates did not result in the production of fermentation inhibitory compounds which were used as culture medium for fermentation without the supplementation of any nutrients. The fermentation results obtained showed that S. cerevisiae presented higher ethanol yields in the MH (>100% as % of theoretical ethanol yield), followed by the results obtained in the CH (87%), and YPD medium (76.4%). The theoretical ethanol yield from 10 g L-1 of glucose results is 5.1 g L 1 of ethanol. The results obtained with the microalgal hydrolysate presenting an ethanol yield beyond the theoretical maximum shows that there are other carbohydrates in the biomass that can be fermented by S. cerevisiae PE-2. Additionally, an optimization of Didymogenes sp. cultivation parameters should be performed to enhance the carbohydrate content in biomass and make it more feasible for 3G bioethanol production. Through the results obtained, it is expected not only to contribute to technical knowledge but to narrow the bottleneck of 3G ethanol production, demonstrating its biotechnological potential.

Keywords: Biofuels, Bioprocess, Biotechnology.

Introduction and Objectives: Brazil, the second-largest ethanol producer globally, faces challenges related to edible sources (1G) and lignocellulosic material (2G), paving the way to 3G bioethanol, which is derived from the hydrolysate photosynthetic microorganisms' biomass, that can thrive without arable land or potable water, relying solely on light, CO2, and nutrients. This project assessed the viability of using distinct photosynthetic microorganisms as feedstock for 3G ethanol production, i.e., a microalgal (Didymogenes sp.) and cyanobacterium (Synechocystis sp.) strains.

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Preliminary conclusions: The theoretical ethanol yield from 10 g L-1 of glucose results is 5.1 g L-1 of ethanol. The results obtained with the microalgal hydrolysate presenting an ethanol yield beyond the theoretical maximum shows that there are other carbohydrates in the biomass that can be fermented by S. cerevisiae PE-2. Additionally, an optimization of Didymogenes sp. cultivation parameters should be performed to enhance the carbohydrate content in biomass and make it more feasible for 3G bioethanol production. Nevertheless, through the results obtained, it is expected not only to contribute to technical knowledge but to narrow the bottleneck of 3G ethanol production, demonstrating its biotechnological potential.

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Chairs: Cristina Fernanda Alves Rodrigues – Renato Gonçalves

Renata de Toledo Cintra
Escola Politecnica, University of Sao Paulo

Abstract Title: Artificial photosynthesis reactions exploring mesoscale 3D printed reactors

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Abstract: One of the main greenhouse gases, in terms of volume, is CO2. Fossil fuels are one of the main causes of environmental problems, which generate climate change and an increase in the planet's average temperature. Due to this enormous global concern, recovering part of the CO2 through chemical reactions, that use sunlight as an energy source, and also producing renewable fuels (such as ethanol, methane, ethanol, among others), is a great opportunity.
The process of artificial photosynthesis, through the conversion of CO2 and H2O into organic products
and oxygen, using metal oxide research and sunlight, is one of the promising and challenging solutions. Therefore, this research is of great relevance to produce clean and sustainable energy. To conduct this line of research, some microstructured reactors were developed, based on previous simulations, so that the geometries of these internal channels could be compared, in terms of efficiency, in a controlled and measurable way. Those reactors prototypes were made with polymers and fabricated through additive manufacturing. A photocatalysis experiment was conducted with reactors of different bases, using ZnO catalyst deposited by spray pyrolysis techniques, on an immobilized translucent surface, aiming to produce organic molecules efficiently.

Keywords: Artificial photosynthesis CO2 reduction Photocatalysis Photoreactor Design
3D printed reactors Solar fuels.

Introduction and Objectives: The objective of this research is to design and manufacture reactor prototypes, focusing on different projects and channel geometries and to experimentally evaluate, in a controlled and optimized manner, the influence of this design on the performance of photocatalysis, with the objective of producing renewable fuels.

Methodology: The prototyping and assembly tests of the reactors were based on a previous simulation work related to this project, where the hydrodynamic flow and the conversion achieved for a model reaction of the reduction of CO2 to CH4 in different channel were studied by computational fluid dynamic simulation (CFD). In this project, combinations of 4 paths and 6 different types of cross sections were made, generating 24 combinations. The ANSYS FLUENT software was used to evaluate the local mixing quality of the reactors (through the velocity perpendicular to the flow), also the reaction conversion rate. Based on simulated results, 4 combinations were considered for prototyping and experimental evaluation. These 4 base models were scaled, designed using Fusion 360 CAD/CAM software (Autodesk, Inc.).

The file was processed for 3D printing in Cura 6.4 software (Ultimaker B.V.). Several printing parameters were adjusted, and the impressions were made with ABS polymer using a printer (Sethi S3, Sethi LDTA) with FDM technology (Fused Deposition Modeling). The 4 sets of reactors were assembled, coupling the base printed in ABS polymer, a sealing blanket in EVA material, a borosilicate glass, and a top also printed in ABS. The assembled set was connected to a peristaltic pump. Regarding the reactor lighting window, borosilicate glasses with a nominal thickness of 2.0 mm were provided. The catalyst was fixed on those glass slides by spray pyrolysis. An aqueous solution of zinc nitrate (0.5M Zn) was sprayed on the surface of

some glass slides, placed one at a time on a heating plate, already preheated to a temperature of approximately 300oC, forming a zinc oxide film (ZnO). All slides were taken to the oven for about 2 hours. Other slides were kept original, without deposition, for comparative effect in the reaction without catalyst. The performance test was conducted with a liquid phase reaction. A solution of acetaminophen (ACT), popularly known as paracetamol, was prepared and placed at the inlet and outlet of the reactor, in a continuous slow flow. The reactor was maintained under UV-A irradiation. Liquid samples were collected regularly, and after analyzed by liquid chromatography, to evaluate the concentration of paracetamol throughout the reaction. An experiment was made with a glass slide without film deposition, and some others with catalyst, with the four different base channels. The channel with best performance in liquid phase was chosen to the following step, gaseous phase photocatalysis. Entry of CO2 and H2O as steam, aiming the production of O2 and organic material, that can be used as renewable fuel. Reaction products analyzed by gas chromatography.

Preliminary results: When performing the photocatalysis with the glass without catalyst, the concentration of the acetaminophen solution remained almost the same, proving that there was no reaction, as expected, indicating the absence of adsorption in the reactor materials and proving its viability for tests with catalyst. Using the glass slide with the oxide film, the results of the chromatography indicated a reduction in the concentration of paracetamol over time, proving that there was a reaction. The rate of consumption of this product was different for each channel, indicating that different flows generate different interactions and results. The gas phase experiment, using the best performing channel, was successful, producing ethane, ethanol, methane and carbon monoxide, as expected.

Preliminary conclusions: It was possible to conclude that channels with a more open cross-section had a greater surface area in contact with UV light, and therefore greater efficiency in the reaction in the liquid phase. The gas phase experiment was successful, producing organic material, as expected.

Rodolfo Lopes Coppo
Institute of Chemistry, University of São Paulo

Abstract Title: Cu-loaded Fe2TiO5 catalysts on CO2 reduction

Authors' Names & Affiliation Institutions of all authors (in order for publication): Rodolfo Lopes Coppo, Institute of Chemistry, University of São Paulo.

Abstract: In this work, Cu-loaded Fe2TiO5 catalysts are investigated for CO2 reduction. Different ratios (%wt) of

Cu:Fe2TiO5 were synthesized, characterized and their performance was evaluated. The objective of this work is to tailor a suitable catalyst to produce high-value-added chemicals through CO2 capture.

Keywords: CO2 capture; pseudobrookite; earth-abundant catalysts.

Introduction and Objectives: Smart strategies for CO2 capture and transformation have been intensified in the past decade to reduce the problems promoted by the greenhouse effect. Photocatalytic processes are advantageous over traditional methods since lead to products obtained at room temperature and atmospheric pressure as well as take advantage of harvesting photons from the sun, an abundant and infinite source of energy. The use of adequate photocatalysts for direct light-driven CO2 reduction plays a major role in the successful obtention of high value-added chemicals with semiconductor oxides, such as titanium dioxide (TiO2), hematite (Fe2O3), bismuth vanadate (BiVO4), and strontium titanate (SrTiO3), typical examples of application in this field.
In particular, the structural and physicochemical properties of perovskites have been investigated for modern applications and the titanate perovskites are photoactive materials with good photostability and corrosion resistance in aqueous solutions. However, their bandgaps are generally above 3 eV, i.e., light absorption occurs mainly in the UV, consequently, these materials need to be improved by modification of their chemical composition through additional oxygen vacancies and element doping to match the visible spectrum. The pseudobrookite, Fe2TiO5, is a hybrid of Fe2O3 and TiO2 that displays a favorable bandgap (~2.0 eV) for visible light absorption with good stability in aqueous solution in a wide pH range, low toxicity, and fast surface reaction kinetics. The use of co-catalysts, such as NiO and Co3O4, in its structure has been proven to enhance substantially the material catalytic activity for water-splitting, for example. Therefore, tailoring the structure of pseudobrookite by loading earth-abundant metals is a low-cost and suitable strategy to increase the availability of photogenerated products. Based on the mentioned above, the objective of this work is expanding the pseudobrookite catalyst application in water-splitting to CO2 capture by obtaining Cu-loaded Fe2TiO5. Materials with different ratios of Cu:Fe2TiO5 were synthesized, characterized, and evaluated for the CO2 reduction reaction.

Methodology: Initially, pseudobrookite (Fe2TiO5) was synthesized by a solvothermal method, reported by Melo et al. (ACS Appl. Nano Mater. 2020, 3, 9303−9317) with modifications, using Fe(NO3)3·9H2O and titanium isopropoxide in isopropanol. The formation of nanoparticles was achieved after calcination at 600 °C. In the following step, copper was incorporated into Fe2TiO5 structure by a solvothermal method using copper acetate as the precursor to produce materials Cu-loaded Fe2TiO5, in proportions varying from 1 to 20% wt Cu.
CO2 reduction was performed in an airtight quartz photoreactor under irradiation with a Xenon lamp. CO2 (5 mL min-1) was bubbled in a suspension containing 25,0 mg of the catalyst in 50 mL of 0,1 mol L 1 NaHCO3 for ~6h. The mixture catalyst + sodium bicarbonate solution was purged with argon (30 mL min-1) for 30 min prior to the reaction. The gaseous products were analysed using an 8890 gas chromatograph (Agilent).

Preliminary results: Results under evaluation.

Preliminary conclusions: Work in progress.

Rosembergue Gabriel Lima Gonçalves
University of São Paulo

Abstract Title: Evaluation of catalysts derived from MgFe-pyroaurite structure impregnated with potassium in the hydrogenation of CO2

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Abstract: In this study, MgFe catalysts derived from the structure of layered double hydroxides (LDHs), enhanced with potassium atoms (K), were investigated in the reverse reaction of the Reverse Water Gas-Shift
(RWGS) reaction. Based on the results obtained, it was observed that the addition of potassium led to a decrease in CH4 production, increasing selectivity towards CO. Additionally, it was demonstrated that the material, when not calcined before the impregnation process with 5% (w.t.) of K, exhibited better catalytic performance than catalysts calcined at 500 and 800°C. Given the unprecedented nature of this research, the present study demonstrates, for the first time in the literature to the best of our knowledge, the most suitable method for preparing

catalysts derived from the MgFe-LDH structure impregnated with K, aiming at CO2 hydrogenation reactions such as RWGS.

Keywords: CO2 hydrogenation, CO, MgFe-based catalysts.

Introduction and Objectives: Anthropogenic emissions of CO2 are recognized as an urgent problem due to CO2 being one of the primary contributors to the Earth's rising average temperature, ocean acidification, and the extinction of certain animal and plant species.

Research into green hydrogen and CO2 as feedstocks for the production of intermediates and molecules of industrial interest, such as CO, methanol, and olefins, is becoming increasingly important. These technologies offer a promising opportunity to reduce CO2 emissions and promote a cleaner and more sustainable economy. Among the products, CO production is crucial for the synthesis of liquid hydrocarbons and other chemicals. However, achieving high selectivity in low-temperature CO production remains a challenge.

To overcome such challenges, this work proposes the use of the three-dimensional and multi-interface structure of LDH as a multifunctional catalyst. The LDH structure provides fundamental characteristics for enhancing the selectivity and stability of the catalyst in the RWGS (Reverse Water-Gas Shift) reaction, such as atomic dispersion and closer proximity of different inserted metals. An LDH of the MgFe type with a molar ratio (M2+:M3+) of 3:1 was selected as a potential catalyst for the RWGS reaction. The choice of magnesium is based on its basic properties, which have the ability to enhance CO2 adsorption near active sites. On the other hand, the choice of iron is due to its nature as a non-noble, low-cost, and widely available metal. Furthermore, a key property of iron in this catalyst is its atomic-level dispersion within the LDH structure. According to the literature, the smaller the iron particle size, the higher the selectivity for CO.

Methodology: The synthesis of the MgFe precursor was conducted as described by Gonçalves et al. [1]. After synthesis, the resulting material was impregnated with 5% (by mass) of potassium (K), both in its as synthesized form and after calcination at 500°C and 800°C in a synthetic air atmosphere. Following impregnation, all catalysts were calcined at 500°C in a synthetic air atmosphere. The obtained catalysts were characterized by X-ray diffraction (XRD), nitrogen adsorption/desorption, and transmission electron microscopy (TEM).

The CO2 hydrogenation reactions were performed in a Microactivity Efficient system from PID Eng&Tech, operated at atmospheric pressure, a gas hourly space velocity (GHSV) of 3600 mL gcat-1 h-1, an H2:CO2 ratio of 3, and a temperature of 370°C. Prior to the reaction process, the catalysts were reduced in a H2 atmosphere (30 mL min-1) at 500°C for 1 hour. The entire reaction line was maintained at 195°C to prevent condensation of reaction products. Conversion values (X%) and selectivity to products were calculated as established in the literature.

Preliminary results: Based on the XRD results, it is possible to observe that the LDH calcined at 800°C exhibits diffraction peaks corresponding to the MgFe2O4 and MgO phases, while the

other catalysts only show peaks of the MgO phase [2]. This observation highlights that, even when derived from the same precursor, the calcination temperature affects the type of phase present in the catalyst during the impregnation with K. The analysis of N2 adsorption/desorption revealed that the MgFe800/K catalyst has a surface area of 44 m^2 g^{-1}, half of the value observed in the MgFe/K and MgFe500/K catalysts, which was 85 m^2 g^{-1}. This result can be attributed to a greater compaction of the structure due to the formation of the $MgFe_2O_4$ phase, as evidenced by the XRD results.
Elemental mapping images obtained through EDX provide clear evidence of the uniform distribution of the elements Mg, Fe, and K throughout the sample, even after the calcination and reduction processes. The results of catalytic activity clearly demonstrate that the addition of K is crucial for increasing the conversion of CO_2 and the selectivity for CO. Additionally, it was determined that the catalyst prepared with K impregnation (MgFe/K) in its as-prepared state is the most advantageous option for the RWGS reaction, as it has a lower cost and shorter preparation time.

Preliminary conclusions: The results obtained demonstrated that the calcination temperature of the precursor directly influences porosity and the formation of the $MgFe_2O_4$ phase. Additionally, it was shown that the LDH structure promotes the uniform dispersion of cations, and the addition of K is important for increasing selectivity towards CO, with no need for prior treatments on the LDH to carry out the impregnation with K.

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Abstract Title: Enhancing Carbonate Formation in Basalts of the Serra Geral Formation

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Abstract: The project consists of conducting experimental mineralisation tests using samples of basalts collected from the Serra geological formation. In this project, the products obtained from the CO2 mineralization reactions will be analysed using characterisation techniques, including controlled mineralisation reactions and characterisation of the products formed in situ within the rock formation. The data collected during this project will be used to experimentally validate previously established rock computational models, thereby helping to elucidate the mineralisation mechanisms. Conventional characterisation techniques such as X-ray diffraction (XRD) and scanning electron microscopy (SEM) were performed to obtain more information about the morphology of the precipitated products. The formation of carbonates, including dolomite and cancrinie, a mixed sodium and calcium carbonate, was observed in two analysed samples.

Keywords: carbonate, carbon dioxide, basalts, carbon capture.

Introduction and Objectives: One of society's foremost challenges is finding ways to reduce atmospheric CO2 emissions. A highly effective approach to address this issue is sequestering this molecule and permanently storing it in geological formations, for example, by storing carbon dioxide in sedimentary basins or transforming it into carbonate minerals. Numerous studies are focused on the example above, as gaseous CO2 can be chemically converted into carbonates relatively simply through a spontaneous and exothermic chemical reaction. This elegant approach mimics natural weathering reactions (chemical reactions between CO2 and silicates containing alkali-earth metals). However, this approach remains challenging for several reasons: (I) the reaction is kinetically unfavourable, (II) high reaction temperatures are required, and (III) continuous mineral consumption is required. In this context, geological CO2 capture provides an alternative to reducing greenhouse gas emissions and replacing products derived from fossil fuels. The use of specific geological formations for geochemical CO2 capture followed by mineralisation is the most promising way to address the long-term emission of this gas. The reactions in this process can take tens of thousands of years, and proposing initially seems unviable. However, recent studies have shown that reactive rocks can dramatically reduce this time frame, taking as little as two years, with a CO2 mineralisation rate of 95%.

Carbon mineralisation processes in rock formations represent a promising strategy. Currently, several initiatives worldwide aim to implement large-scale geological storage of CO2. Research into inorganic carbon storage primarily focuses on sequestering CO2 in underground geological formations, such as (I) saline aquifers, (II) depleted oil and gas fields, and (III) unmineable coal deposits. The advantage of this geological sequestration method is its relatively low cost when separated from CO2 capture, separation, and transportation. However, some potential issues associated with sequestration in geological formations include (I) permanence, (II) long-term monitoring, (III) verification, and (IV) enhanced environmental risks, along with other potential secondary risks. An alternative to conventional geological CO2 sequestration is inorganic carbon mineralisation, where CO2 reacts with metal cations to form carbonate minerals.

In this context, the primary aim of this project is to investigate mineralisation in basaltic rocks of the Serra Geral to achieve controlled carbonate formation. The significance of carbonate reactivity is pivotal in such reactions, as it directly influences the efficiency of the process, utilising characterisation techniques to verify the formation of these carbonates.

Methodology: We are particularly interested in the rock formation of Serra Geral. The Serra Geral is a highly significant geological volcanic outcrop in eastern South America. It results from two igneous phases with extreme ages ranging from 153 to 115 million years ago (Ma). The Serra Geral formation consists of flows of tholeiitic basalts of the augite type and their associated bases. Its texture is generally compact. Regions with a high composition of Anorthite (calcium plagioclase) ranging from 48 to 50%, Augite (calcium pyroxene) from 20 to 30%, and Pigeonite (pyroxene without Ca) at ~4% are extremely interesting for mineralisation reactions, as their abundance of divalent cations would facilitate such reactions. Initially, samples collected from outcrops in the Serra Geral rock formation would undergo mineralisation reactions using CO2 as a carbon source to form carbonates. The basaltic samples would be characterised and subsequently used as a source of ions to carry out the mineralisation reactions. First, a peristaltic pump would inject 100 ml of 1M NaCl solution into a column containing basaltic samples. This reaction mixture would be continuously introduced into 100 ml of 1M NaOH solution, while CO2 would be injected under the control of a flow meter. The products of these solutions are filtered and washed.
A comprehensive methodological study encompassing the adjustment of reaction conditions (time, temperature, pressure, and fluid concentration) becomes necessary to investigate the mechanism of particle formation. Techniques for characterising the products formed through CO2 mineralisation reactions are essential for elucidating the structural characteristics of the carbonate species obtained. One of the critical techniques for structural characterisation is X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM); this microscopic method aims to produce high-resolution images of the surface of a given sample, providing crucial insights into the morphology of the obtained products. Other characterisation techniques that can also be employed to gather information about the prepared products include Infrared Spectroscopy (IR), Raman Spectroscopy, Atomic Force Microscopy, Fluorescence Microscopy, Energy-Dispersive X-ray Spectroscopy, Thermogravimetry, X-ray Tomography (XRT), and Mercury Intrusion Porosimetry (MIP). This array of techniques is valuable for obtaining a comprehensive characterisation of carbonates obtained through CO2 mineralisation reactions, contributing to the development of the research project and assisting in the theoretical approach to investigating the mechanical aspects of the mineralisation process.

Preliminary results: Mineralisation tests were conducted on four specific types of basalt samples representing different rock outcrops of the Serra Geral. These samples are referred to as BORB, CARR, IND, and CGS. The formation of insoluble precipitates, such as calcium and magnesium carbonates, was observed in the first two samples. In the last two samples (IND and CGS), a white, insoluble precipitate in water was noted, possibly indicating carbonate formation. In the IND sample, it was possible to identify the presence of a phase of a

feldspathoid carbonate called cancrinite, with the molecular formula Na6Ca2[(CO3)2Al6Si6O24] 2H2O. The formation of this sodium carbonate is explained by the high amount of NaOH present in the solution, as an increase in pH is necessary for dissolution reactions to occur. It is initially required to obtain a known carbonate called dawsonite to form cancrinite. Therefore, it can be concluded that dawsonite is formed and rapidly consumed to obtain cancrinite, as no dawsonite phase was found in the IND sample after injection. In the CGS sample, the presence of a dolomite phase was identified. This discovery suggests the formation of carbonates that incorporate magnesium into the calcite mineral or possibly the presence of dolomite, a mineral composed of calcium and magnesium carbonate. Detecting this magnesium carbonate phase is relevant for understanding the mineralisation process in the sample, indicating the incorporation of magnesium cations into its structure and contributing to knowledge of the chemical transformations that occurred during the CO2 mineralisation reaction.

Thermogravimetric analyses performed on the CGS and IND samples revealed significant differences in the thermogravimetric curves before and after the mineralisation process. The curves obtained before and after mineralisation showed distinct patterns, providing direct evidence of carbonate formation. Specifically, a significant mass loss of around 550°C was observed, indicating the thermal decomposition of the formed carbonate. Approximately 3% of the mass was lost as carbonate in the CGS sample, while in the IND sample, this loss was estimated to be about 1%. These results support the effectiveness of induced mineralisation in the samples, confirming carbonate formation as one of the leading products resulting from the process, with distinct variations between the samples. Through scanning electron microscopy (SEM), it can be confidently asserted that the mineralised carbonate was indeed iron-rich dolomite. Dolomite exhibits distinctive characteristics when observed via scanning electron microscopy (SEM), including a crystalline structure, granular surface, chemical composition rich in calcium, magnesium, and carbon, distinct cleavage, and colour variation.

Preliminary conclusions: The CO2 mineralisation tests conducted at the laboratory scale have significantly improved our understanding of cation exchange reactions and precipitate formation in different basalt samples from the Serra Geral region. Identifying the mineral phases of cancrinite and dolomite in the IND and CGS samples has provided valuable insights into the mechanisms involved in CO2 mineralisation.

These findings indicate the incorporation of magnesium cations and the formation of carbonates, contributing to the comprehension of the chemical processes occurring during mineralisation. BET experiments allowed for the analysis of the porosity of the CGS and IND samples, demonstrating that both are non-porous materials with a solid surface lacking significant pores.

This information is relevant for future studies involving adsorption and porous surfaces. The SEM analyses of the CGS samples revealed a considerable presence of minerals, including pyroxenes, diopsides, anorthite, and magnesite, providing valuable information about the mineralogical composition of the sample and its geological relevance.

The mineralisation yields in the CGS and IND samples were generally satisfactory, with 60%

and 14% rates, respectively. The difference in calcium and magnesium concentrations can be attributed to vesicles in the CGS sample, underscoring the importance of detailed sample analysis. These results contribute to a more comprehensive understanding of mineralisation in various geological contexts.

Sergio Brochsztain
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Abstract Title: Naphthalenediimide-containing metal-organic frameworks for mixed matrix membranes designed for CO2 separation

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Abstract: Novel materials based on aromatic imides will be synthesized, with applications for the energy sector. The proposal aims the synthesis of N,N′-bis(4-carboxyphenyl)-1,4,5,8-naphthalenediimide (CNDI), featuring carboxylate ligands. The compound will be reacted with either zinc or zirconium salts, to give metal organic frameworks (MOFs), which will be employed for the CO2/CH4 separation. For this purpose, mixed matrix membranes (MMMs) will be prepared, containing the obtained MOFs embedded into a polymer matrix (polyetherimide or polysulfone). The permeability and selectivity of the MMMs towards the different gases involved in CO2 capture will be measured.

Keywords: Carbon Capture; Metal Organic Frameworks; Aromatic Imides; Mixed Matrix Membranes.

Introduction and Objectives: According to the Intergovernmental Panel on Climate Change, climate changes caused by human activity are leading to more frequent and extreme weather events. These climate changes have been attributed mainly to an increase in the emissions of CO2. In this context, it is very important to find new materials for the capture and storage of CO2. These materials should perform gas separations, such as CO2/N2 in the exhaust of thermoelectric stations and should therefore display high selectivity and permeability for gas separation. One technology that has been considered for this purpose is the use of mixed matrix membranes (MMMs), which consist of a polymeric matrix impregnated with an inorganic filler, such as metal-organic frameworks (MOFs). MOFs are porous crystalline solids formed by nodes, which are metal cations, interconnected by bifunctional organic ligands. The main goal of the present work is the synthesis of MOFs for MMMs, using 1,4,5,8-naphthalenediimides (NDI) as the organic ligands. Herein, we present a novel NDI ligand, CNDI, containing carboxylic acid ligands.

Methodology: CNDI was synthesized by the reaction of 1,4,5,8-naphthalic dianhydride with 4-aminobenzoic acid, using molten imidazole as the solvent. Two types of MOFs were prepared using CNDI as the ligand, namely an IRMOF, employing Zn as the cation, and an UiO-type MOF, employing Zr as the cation. MOF syntheses were performed in an autoclave, using dimethylformamide as the solvent. The MOF were characterized by X-ray diffraction, scanning electron microscopy and N2 adsorption isotherms.

Preliminary results: The CNDI-based UiO MOF showed higher crystallinity, also presented mesoporosity, leading to the conclusion it can be a candidate to be used in the synthesis of MMM.

Preliminary conclusions: The new ligand CNDI has a great potential for MOF construction

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Abstract Title: Scale-up study of a pressurized reactor for converting CO2 to methanol

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Abstract: We investigated the scale-up of a reactor used in the catalytic conversion of CO2 to methanol under supercritical conditions. This study simulated the reactor, designed to produce 1Nm³/h of methanol using the Aspen Plus software and the PFR (plug-flow reactor) block. Furthermore, the parameters of the exchanger's cooling jacket were calculated, which was modelled as a double-tube heat exchanger, obtaining the thermal load, and the water flow required for cooling, in addition to the surface area of heat exchange. heat. The global heat exchange coefficient (U) was also estimated taking into account the composition of the reaction medium and the reactor material. Preliminary results show that a water flow of 0.121 l/min is necessary to maintain the reactor at 200 °C.

Keywords: CO2 abatement, methanol, process simulation, supercritical flow.

Introduction and Objectives: New CO2 emission reduction technologies are necessary to restrain the escalated climate change. To avoid global heating exceeding 2.0 °C, i.e., for maintaining a CO2 atmospheric concentration of 450 ppm, an amount of 120 to 160 Gt of CO2 must not be emitted until 2050 [1,2]. Thus, designing a large scale and profitable process of CO2 utilization is necessary to reach the climate goals and also to create a carbon-based circular

economy.
In this context, our research group has developed an efficient supercritical flow process for the catalytic conversion of CO2 into methanol. The studied ReOx/TiO2 catalyst presented 98 % selectivity to methanol, CO2 conversion of 18% at 200 °C and 100 bar, with CO2:H2 of 1:4 [3]. To carry out a scale-up of the process to an industrial scale, a pilot plant with 1Nm²/h of methanol production capacity must be previously designed and constructed. The assessment of the reactor, the industrial process core, is crucial to assure a stable conversion process, with high conversions and selectivity.
This study focused on the simulation of a reactor for the pilot plant, aiming a 1Nm³/h methanol production.

Methodology: The scaled-up reactor was modeled in two steps using the commercial software Aspen Plus 8.1 using the SRK EOS thermodynamic model modified by Mathias [4]. The first step consisted of modeling the reaction using a plug-flow reactor (PFR) block, to estimate the thermal load and the temperature profile along the reactor length. With these first results, it was

possible to carry out the second step, in which the cooling system was modeled as a double-tubed heat exchanger. The heat exchanger area, water flow, and global heat exchange

coefficient was calculated. A flow of H2 and CO2, in a molar proportion of 1:4, was considered. The cooling system was modelled considering that the temperature of the reaction must be 200 °C and an inner pressure of 100 bar. Subcooled water at 15.6 bar and 195 °C was chosen as the cooling fluid. The reaction kinetics were represented using copper-based catalyst kinetics [5], as reported in the literature [4].

Preliminary results: The PFR block results, obtained during the Aspen Plus simulation, showed the temperature profile. During the length of 0.3 m, the temperature profile increased from 200 °C to 300 °C, confirming the necessity of a dedicated cooling system. With the heat load calculated using this temperature increase, a counter current double-tubed heat exchanger was calculated to emulate the cooling jacket. The inner exchange area was estimated to be 0.005 m² and the needed flow of cooling water was 0.121 l/h.

Preliminary conclusions: The Preliminary conclusions showed that the cooling jacket system is necessary to maintain the reactor temperature at 200 °C. The inputted kinetics from the literature showed good agreement with what was expected from the experimental data. The reactor temperature profile guided the ongoing heat load calculation and heat exchange area preliminary estimation. All the results are going to be compared to the literature reports for validation.

Vinicio Simizu
IQ-USP

Abstract Title: Tailoring Pd and Fe Catalysts for Ethanol Synthesis in CO2 Hydrogenation

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Abstract: The study aims to valorise carbon dioxide (CO2) by converting it into high-value alcohols for the industry, such as ethanol and propanol. The central challenge lies in finding catalysts that enable this conversion, particularly for ethanol, given the stability of the CO2 molecule. A bimetallic catalyst was developed with
palladium (Pd) and iron (Fe) adsorbed on TiO2, with Pd being responsible for the initial step of transforming CO2 into carbon monoxide (CO), and Fe for the subsequent reduction of CO into ethanol. Different synthesis techniques and salt addition sequences were explored to optimize the selectivity of the reaction. The catalysts were tested under controlled conditions, resulting in varying selectivity's for the final products. Notably, the coprecipitation of Fe and

Pd increased selectivity for methanol. Catalysts containing only K and Fe exhibited high CO2 conversion and increased C-C coupling, with 20.28% selectivity for ethanol among alcohols.

Keywords: heterogeneous catalysis, CO2 valorisation, coprecipitation, deposition-precipitation.

Introduction and Objectives: One of the biggest challenges humanities currently faces is climate change. Earth's temperature has risen approximately 2 degrees Celsius since the pre-industrial period (17th century) to the present day, and it could increase by another 2 degrees in the coming years if nothing is done to reverse this scenario of global warming. According to the United States National Research Council, the accumulation of greenhouse gases, such as carbon dioxide (CO2), is responsible for both the rise in atmospheric and ocean surface temperatures.
In addition to reducing worldwide CO2 emissions, other alternatives have also been proposed, including smart solutions to decrease CO2 levels, covering both capture and utilization. This work aims to valorise CO2 by converting this greenhouse gas into industrially valuable products, also known as high-value products. In this case, the main goal is its conversion into higher alcohols, such as ethanol, 2-propanol, propanol, and butanol, for example, though molecules like methanol are also acceptable.
The main challenge of this work is to select and adapt catalysts that meet the goals of CO2 valorisation, such as high conversion and selectivity for some of the higher alcohols, especially ethanol. Due to the stability of the CO2 molecule, the material must be suitable for thermocatalysis under high pressures, thus enabling its hydrogenation into the desired product.

Initially, the catalyst was designed to operate in two stages. The first is responsible for the hydrogenation of CO2 into carbon monoxide (CO), a process also known as Reverse Water-Gas Shift (RWGS), and the second stage should be capable of reducing CO into ethanol. Therefore, a bimetallic catalyst was designed to meet these two needs, using palladium (Pd) as the first metal due to its ability to generate CO, and iron (Fe) as the second metal, known for its capacity for C-C coupling in Fischer Tropsch reactions.

Methodology: As explained earlier, Pd and Fe are crucial species for this study, where catalyst design poses the greatest challenge. So far, a series of materials have been developed for this purpose, ranging from synthesis techniques to the order of adding precursor salts. This way, the expectation was to understand how to increase the selectivity of the reaction for higher alcohols, taking into account the distribution of metals on the catalyst surface and their interaction with the support, TiO2.
For the Pd-based catalysts (5% wt), the metal was adsorbed onto TiO2 through pH-induced deposition precipitation. On the other hand, the Fe-based catalysts (5% wt) were prepared through wet impregnation, in a step independent of Pd, and could be added either before or after, depending on the synthesized material. In some cases, K (3% wt) was also added through impregnation as a promoter for C-C coupling. Each synthesized material was dried in an oven at 120°C and thermally treated in a flow of N2 at 500°C for 3 hours, subsequently.
The tested catalysts (10g) were reduced in a flow of H2 (1ml.min-1) at 500°C for 30 minutes. After this procedure, each of them underwent catalytic tests, using stainless steel batch reactors (10ml) in a gas mixture at 100 bar (H2/CO2:3) for 17 hours at 250°C. At the end of the reaction, the products were analysed in two parts. One of them consists of a gas sample collected to identify the products that are gases at room temperature. The other part consists of the products that are liquid at the same temperature, extracted through solubilization of the remaining gas content from the reactor in cold water.

Preliminary results: Overall, the order of impregnation of Fe in relation to the deposition of Pd onto TiO2 does not significantly impact the result of CO2 hydrogenation, maintaining the conversion and selectivity values. On the other hand, the order in which K is impregnated alters the catalyst's behaviour, increasing selectivity for methanol when K is added to the support before Pd. Additionally, when the catalyst contains only K and Fe impregnated on TiO2, there was higher CO2 conversion and an increase in C-C coupling, with a selectivity of 20% for ethanol among the alcohols (1% among all products). In contrast, the selectivity of the alcohols dropped from 30% to 7%. On the other side, a satisfactory amount of methanol was produced through Pd-Fe coprecipitated catalyst, with selectivity of 45% e CO2 conversion of 21%. Another major product is CO, an important subtract that can be recycled and produce more methanol.

Preliminary conclusions: Individually, Fe/TiO2 and Pd/TiO2 exhibit similar behaviour to FePd – low CH4 and good alcohol production. The co-precipitation [COP] of Fe and Pd enhances conversion and selectivity towards alcohols, especially methanol. PdFe/TiO2 [COP]

is intriguing due to its simultaneous production of CO alongside methanol, which could be recycled. FeK/TiO2 performs best for ethanol, where K promotes C C coupling. However, methanation in FeK/TiO2 remains predominant.

Vinícius da Costa Santos
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Abstract Title: Synthesis of ammonium perrhenate supported catalyst

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Abstract: Rhenium catalysts have been gaining prominence in the CO2 hydrogenation reaction due to their high selectivity for alcohol formation, specifically methanol. Ammonium perrhenate, the most abundant rhenium compound, makes its use in catalysis economically

advantageous. When combined with a rare earth metal and a support known in the literature for its high CO2 conversion rate, namely titanium dioxide, it broadens the scope of this work. The objectives are to investigate the calcination temperatures (250°C, 300°C, and 350°C) of the catalyst, with 1 wt% of active metal, in a horizontal tubular furnace under synthetic air flow, comparing the results of CO2 conversion in both non-calcined and calcined catalysts, as well as the selectivity of products, conducted in a batch reactor under supercritical CO2 conditions. At high temperatures and in an oxidizing atmosphere, ammonium perrhenate decomposes into rhenium oxide, an inorganic compound known in the literature for its high CO2 conversions and selectivity towards methanol. The non-reduced catalyst achieved a CO2 conversion of 2.35%, methanol selectivity of 55.95%, methane selectivity of 41.77%, and CO selectivity of 2.09%, while the catalyst reduced at 250°C showed a CO2 conversion of 1.84%, methanol selectivity of 59.65%, methane selectivity of 29.53%, and CO selectivity of 10.74%. The low conversion is expected due to the small catalyst mass, but the reduction of the catalyst at high temperatures in a synthetic air flow has shown an increase in methanol and CO selectivity, which are intermediates in the CO2 hydrogenation to methanol reaction, while reducing methane selectivity, the most highly reduced carbon molecule. In future reactions, it is expected that catalysts calcined at higher temperatures will produce more intermediates and methanol itself, reducing methane formation.

Keywords: Conversion of CO2; Supercritical CO2; Rhenium; Methanol; Catalysis; Synthesis.

Introduction and Objectives: Rhenium catalysts have been gaining recognition in the CO2 hydrogenation reaction due to their high selectivity for alcohol formation, particularly

methanol. Ammonium perrhenate is the most abundant form of rhenium, making it economically advantageous for catalysis. Combining a rare earth metal with a well-known CO2 conversion support, titanium dioxide, broadens the scope of this study. The objectives include investigating the reduction temperatures (250°C, 300°C, and 350°C) of the catalyst in a horizontal tubular furnace under synthetic air flow and comparing the results of CO2 conversion and product selectivity with those obtained in a batch reactor under supercritical CO2 conditions.

Methodology: The catalyst synthesis involves wet impregnation, where ammonium perrhenate (Mollymet®) is dissolved in deionized water to achieve a sufficient mass for 1 wt% of active metal. This solution is stirred in an Erlenmeyer flask with magnetic agitation for an hour. Subsequently, the solubilized volume is added to a volumetric flask containing Degussa P25 titanium dioxide® and left under magnetic agitation for twenty-four hours. After the impregnation process, the solution in the flask is transferred to a rotary evaporator and rotated at 70°C and 80 mbar vacuum until complete water evaporation. The impregnated catalyst powder is placed in a ceramic boat for combustion in a horizontal tubular furnace under synthetic air flow, with temperature ramps of 10°C/minute until reaching the programmed temperature (250°C, 300°C, and 350°C). The catalyst is then reduced for one hour and cooled down. The unreduced catalyst and those reduced at the studied temperatures are weighed (10 mg) and placed in a CITUA® batch steel reactor, with 80 bar of hydrogen gas and 20 bar of carbon dioxide gas. They react for 20 hours at 200°C. After the reaction, the gas phase is analysed using a Gas Chromatograph with Thermal Conductivity Detector (GC-TCD), and the liquid phase is dissolved in 2 mL of deionized water and analysed using a Gas Chromatograph with Flame Ionization Detector (GC-FID).

Preliminary results: The unreduced catalyst achieved a CO2 conversion of 2.35%, methanol selectivity of 55.95%, methane selectivity of 41.77%, and CO selectivity of 2.09%. The catalyst reduced at 250°C achieved a CO2 conversion of 1.84%, methanol selectivity of 59.65%, methane selectivity of 29.53%, and CO selectivity of 10.74%. Further batch tests of the catalysts reduced at 300°C and 350°C will be conducted, along with ICP-OES and XRD characterizations of the four powder catalysts.

Preliminary conclusions: The low conversion is expected due to the small amount of catalyst used. However, reducing the catalyst at a high temperature and under synthetic air flow has shown an increase in methanol and CO selectivity, which are intermediates in the CO2 hydrogenation to methanol reaction, while reducing methane selectivity, the most highly reduced carbon molecule. In future reactions, it is expected that catalysts calcined at higher temperatures will produce more intermediates and methanol itself, reducing methane formation.

0811 - PS16 (TV4)
Chairs: Maurício Salles – Renato Monaro

Marcel Augusto Alvarenga Viegas
Universidade de São Paulo

Abstract Title: Smart and Sustainable Electric Vehicle Fast Charging Station

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Abstract: This work aims to contribute to the development of a possible Brazilian standard for a Smart and Sustainable Electric Vehicles Fast Charging Station, with a topology that allows interconnection: Photovoltaic Generator (PV); Stationary Batteries (BE); Electrical network; DC bus; Electric Vehicle; Power Switches; DC-DC Converters (Buck, Boost, and Bidirectional Converter); AC-DC Bidirectional Converter; High Frequency Transformer; Matrix Converter and LCL Filter, with its respective control loops. And through dynamic analysis and the proposition of control strategies for power converters, adapt the Charging Station to the Brazilian reality in terms of voltage, current, frequency and other parameters established by international standards. The system's power and control designs were carried out through

calculations and validated through simulations. The simulations will be carried out using MATLAB/Simulink software. The methodology will be divided into 2 stages: an off-line stage in which five (5) operational scenarios will be created, which will serve to build a database, where the use or not of the Electric Grid will be analyzed, according to the intermittency of the Photovoltaic Generator, the State of Charge (SOC) of the Stationary Batteries and the Electric Vehicle. And a second stage in real time, which is one of the main contributions of this work. At this stage, an intelligent Fuzzy Supervisor was proposed, which will manage the operating modes of this Microgrid and the balance of power flow between its components.

Keywords: Smart and Sustainable Eletric Vehicles Fast Charging Station, Photovoltaic Generator, Stationary Batteries, Power Switches, Fuzzy Supervisor.

Introduction and Objectives: A new paradigm in the electricity sector has been established over the last few years, through the concept of Smart Grid (SG). Mainly due to the following aspects: growing demand; technological advancements; environmental, social and economic barriers imposed on the construction and expansion of the electrical energy system to meet the growing consumption of electrical energy; and growth of Distributed Generation (DG). This research has the general objective of developing a proposal to contribute to the adoption of a Brazilian standard for a Smart and Sustainable Electric Vehicle Fast Charging, with a topology that allows interconnection: Photovoltaic Generator (PV); Stationary Batteries (SB); Electrical

Grid; DC bus; Electric Vehicle; power switches; DC-DC converters (Buck, Boost, and Bidirectional Converter); Bidirectional AC-DC converter; High Frequency Transformer; Matrix Converter and LCL Filter, with their respective control loops.
And, through dynamic analysis and the proposition of control strategies for power converters, differentiate this project from the North American, European and Asian standards available in the literature and on the market and, in this way, adapt the Charging Station to the Brazilian and South American realities in terms of voltage, current, frequency and other parameters established by international standards.
Furthermore, the proposed topology has an intelligent Fuzzy Supervisor that

will manage the operating modes in real time and will be responsible for balancing the power flow between the DC bus, sources and loads, so that it can provide the
best setpoints for the Microgrid components depending on the availability of

sources and load needs, thus not violating operational limits.

Aiming to achieve the general objective, requirements for the system will be proposed, based on examples from the literature, proposing adjustments to the topologies used to form each subsystem. Reviews will be made on the functioning of topologies and their
design equations, with which the computational simulations will be carried out. The power and control project of the plant's components will be presented, so that in the future, if possible, a prototype can be created. The specific objectives of this work are:

- Propose a contribution to Microgrid topologies dedicated to fast charging of Electric Vehicles (EV); - Design all components of this Microgrid and their respective controls;

- Carry out simulations of various operating scenarios, considering the intermittency of the Photovoltaic Generation, the State of Charge of the Stationary Batteries and the Electric

Vehicle, in addition to the possible use of the Electric Grid, depending on the time and/or operating conditions of the other components the Microgrid;

- Design a Fuzzy Supervisor that will be responsible for managing power flows in the Microgrid and better take advantage of the available resources of sources and loads, as well as provide the setpoints for them.

Methodology: Studies were developed with the Fast-Charging Station proposal. All components of the system, in principle, were designed and simulated separately to validate their proper functioning, and later linked together. For this, the Simpowersystems tool associated with Simulink® was used, which accompanies the MATLAB® software, the version used was R2016a.

5 simulations of operating modes were carried out for the Microgrid under study: in Mode 1 the PV Generator provides energy to the Stationary Batteries (SB), to the Vehicle Electrical and for the Electrical Grid; in Mode 2, the Stationary Batteries supply energy to the Electric Vehicle;

in Mode 3 there is no photovoltaic generation available and the Electric Grid supplies energy for both Stationary Batteries and the Electric Vehicle; in Mode 4 the
PV Generator provides energy only to the Stationary Battery Bank, considering that the Electric Vehicle is charged; and in Mode 5 it is also considered that the Electric Vehicle is charged and that the Photovoltaic System will supply the Electric Grid and Stationary Batteries.

Preliminary results: The method consists of two stages, an offline stage and a Real-Time stage.
In the offline stage, a Database is built using power flows originating from the opening and closing of power switches according to the availability of sources and loads; Once you have this data, calculations will be made to obtain the input variables from the Fuzzy Supervisor who will be responsible for decision making in the Real Time stage and will therefore define the best operating points for the Microgrid components. The Operating Modes of the proposed Charging Station for energy management will be carried out by opening and closing the power switches from CH1 to CH8, which, depending on the Operating Mode, will or will not allow power flows from one component to another of the system. Some variables will be important in this algorithm, such as: State of Charge of Stationary Batteries (SOCBAT); State of Charge of the EV battery (SOCEV); voltage and current of Stationary Batteries (VBAT and IBAT, respectively); DC Bus voltage and current (VDC and IDC, respectively); voltage and current of the Electrical Grid (Vgrid and Igrid, respectively). These Operation Modes will constitute the offline stage and will serve to build a Database, which will be given as input for the Fuzzy Supervisor to carry out decision making in the Real Time stage.

Preliminary conclusions: In this work, the design and computational dynamic analysis of a smart fast charging station for electric vehicles. Proven by results, an advantage was obtained over other topologies in the literature in terms of efficiency, since the topologies compared to this study present efficiencies in relation to processed power close to 82%, without considering the transformer, and this work considered the use of transformer in all simulations, in which an average efficiency was obtained in relation to the processed power for the 5 simulated scenarios of 87.578%. Another important contribution of this study is the proposition of a Fuzzy Supervisor low complexity for charging and discharging lithium-ion batteries. It is observed that the battery is charged when energy is available and is discharged if the demand exceeds the energy generated. The fuzzy model, which has 25 rules with two inputs (ΔSOC and PBalance) and one output (IBat), is used to control battery charging/discharging. The results prove the effectiveness of the proposed topology, since all values for the variables Voltage, Current and State of Charge of Stationary Batteries and Electric Vehicle are within the operating ranges. The results of this work will be applicable mainly in the electrification sector of transport, with strong potential for insertion of the proposed technology in the EV charging infrastructure, EV batteries and EV charging management software. The proposed methodology can be used by companies in the electrical sector in the simulation of events in permanent and transient regime for analysis of the operation of charging stations in general.

Matheus Batista Cordeiro de Souza
USP

Abstract Title: Parametric study of an ethanol-based solid oxide fuel cell

Authors' Names & Affiliation Institutions of all authors (in order for publication): Matheus B. C. de Souza; T. Lopes; J. Meneghini.

Abstract: One of the technologies capable of reducing CO2 emissions from the transport sector are the solid oxide fuel cells (SOFC). These devices operate on high temperatures, and are capable of converting any fuel cell source that can be electrochemically oxidized into electricity, and can be readily used in electric vehicles. Of particular interest is feeding them with ethanol fuel, where the logistics network for operation and distribution is already established. In this work we have developed an electrochemical model to study the current-voltage characteristics of a SOFC. This model consists on a set of analytical equations based on Fick's model, Ohm's law and the Butler-Volmer equation. The fuel used on the anode side is considered to be a mixture of ethanol, steam and an inert carrier gas, of which we have studied its thermodynamic equilibrium in ranges of water-to-ethanol ratio from 0 to 7, and temperature from 550 to 900 °C, in line with operational limitations of the cell.

Keywords: SOFC; Ethanol; Electrochemical model.

Introduction and Objectives: Solid oxide fuel cells are a promising and efficient energy conversion technology, and have garnered significant attention due to their ability to directly convert chemical energy into electricity with high efficiency, low CO2 emissions and a wide range of applications, both stationary and in transportation. To harness their full potential and optimize their performance, it is crucial to combine experimental testing, which are often lengthy in duration, with numerical models, to understand the complex electrochemical processes taking place within these devices. This work aims to develop a combined model for ethanol based SOFCs, where not only the electrochemical processes within the cell are studied, but also the thermodynamics of ethanol steam reforming, with the ultimate goal of optimizing both operational parameters of the device and fuel conditions.

Methodology: The thermodynamics of ethanol steam reforming was studied using the DWSIM open-source chemical process simulator, where equilibrium thermodynamics was calculated. using the nested loops numerical approach. The electrochemical model of the SOFC was idealized based on a combination of Ohm's law for the overpotential calculations, the Butler-Volmer equation for the current-voltage relations, and Fick's model in combination with Knudsen diffusion to correct for diffusion within the porous electrodes.

Preliminary results: Results for the modelling of ethanol steam reform show that in our operational conditions no ethanol is ought to reach the SOFC, but instead a mixture of H2, H2O, CO, CO2 and CH4. In the SOFC the principal species to the fuel stream is the H2 content, and we were able to see that it decreases with increasing steam and carrier gas content, and increases with operating temperature. Graphite formation, the main poisoning species, as it clogs the pores of the SOFC, decreases with increasing steam and operating temperature. In the electrochemical model, several considerations have to be made, mainly that the fuel inlet is a binary mixture of H2 and H2O, as we currently have no means of modelling the mass transport of a multicomponent gas mixture. In addition, we have to consider that only H2 and H2O on the anode side, as well as O2 on the cathode, are the reacting species.

Preliminary conclusions: In our operating conditions, the anode fuel to the SOFC is ought to be a mixture of five different species, which we currently have no means to model the mass transport through Fick's model, so it is approximated as a binary mixture of H2 and H2O. In a Preliminaryy model, these species, along with O2 on the cathode side, are the ones responsible for changing the cell potential according to the Nernst equation, whereas in actual measurements the other three anodic species also affect the cell voltage. In the next steps, we will continue to improve our model, ultimately creating a 0D stationary model, and later developing a 1D SOFC model to study temperature and concentration-dependent phenomena.

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Abstract Title: Cost Modelling of LFAC Transformers: Insights and Implications

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Abstract: The shift towards Low Frequency Alternating Current (LFAC) transmission systems has brought about its own set of challenges, particularly concerning the associated transformer equipment. LFAC-based transformers are distinguished by their size, due to the requirement of increased dimensions and weight at reduced operational frequencies. This work explores the cost functions associated with LFAC transformers, emphasizing their contrasts with standard HVAC systems. Leveraging established cost functions and integrating frequency-dependent modifications, we draw upon mathematical models to elucidate the economic implications of LFAC technologies.

Keywords: Low Frequency Alternating Current (LFAC), Transformer Costs, HVAC, Offshore Wind Farms (OWFs), Transmission Systems, Cost Functions

Introduction and Objectives: In recent years, the energy landscape has undergone significant transformations, notably with the push towards renewable energy sources and the adoption of advanced power transmission technologies [1]. One such emerging technology is the Low Frequency Alternating Current (LFAC) transmission system. Primarily explored for offshore wind farm power transmissions, LFAC systems promise numerous advantages over traditional methods [2]. While they serve functions akin to their High Voltage Alternating Current (HVAC) counterparts, The inherent variances in LFAC transformers can have an impact on design, operational methods, and, most importantly, the economic measures connected with their deployment [3]. As the frequency of operation is reduced, transformers inherently require larger sizes, directly influencing their cost structures [4]. This change poses both technical and financial challenges, making it paramount for stakeholders to comprehend and quantify these implications. This study delves deep into the intricacies of LFAC transformers, focusing on their cost functions, and attempts to provide a comprehensive mathematical model that captures the economic nuances of employing LFAC technologies.
Objectives:

• To understand the impact of operating at lower frequencies on transformer sizing and costs. • To establish a mathematical model that describes the cost functions for LFAC transformers.

Methodology: This study initiated with a comprehensive examination of the well-established cost functions pertaining to HVAC systems. This foundational step provided a benchmark for discern This study initiated with a comprehensive examination of the well-established cost functions pertaining to HVAC systems. This foundational step provided a benchmark for discerning the differences introduced by LFAC operations. Subsequently, we turned our attention to the unique frequency-dependent attributes of LFAC. By embedding these parameters into our model, we captured the intricate relationship between frequency and transformer VA ratings.
To ensure our model's accuracy and relevance, we embarked on a comparative analysis using data from existing literature. This not only validated our findings but also identified areas of

potential refinement. Through this streamlined approach, we aimed to shed light on the economic dynamics of LFAC transformers and their implications in the energy sector.

Preliminary results: Our ongoing investigation into LFAC transformers has yielded some initial insights. It is becoming evident that when these transformers operate at lower frequencies, there's a trend towards an expansion in their physical dimensions. This shift has potential economic ramifications, especially when transitioning from traditional HVAC systems to LFAC setups. An intriguing pattern has also emerged, indicating a direct relationship between a transformer's operational frequency and its VA rating. While these insights provide a foundational understanding, a comprehensive cost model is still under development, aiming to shed further light on the full spectrum of economic implications.

Preliminary conclusions: As the energy sector leans into LFAC transmission systems, notably for Offshore Wind Farms (OWFs), understanding the intricacies of transformer economics becomes utmost importance. Preliminaryy indications suggest that the increase in transformer size due to reduced frequencies could substantially influence cost structures. While our in-depth study is in its initial stages, the initial insights already underscore the need for a comprehensive cost function model tailored for these LFAC transformers. As we progress, our research aims to shed light on these aspects, ensuring stakeholders are equipped with actionable insights to navigate the evolving landscape of LFAC technologies.

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FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Themes and perspectives in Agri-PV research: a global bibliometric analysis showcasing its relevance and importance to energy transition.

Authors' Names & Affiliation Institutions of all authors (in order for publication) *[1]Escola Superior de Agricultura Luiz de Queiroz (ESALQ); [2]Instituto de Energia e Ambiente da USP(IEE)

Abstract: The growing global demand for food and energy drives changes in land use. In this

context, agri-PV is a land use hybridization method that can increase land use efficiency, combining photovoltaic generation with productive uses such as agriculture, livestock and ecosystem services, among others. This work carries out a bibliometric evaluation on the agri-PV theme and seeks to present an overview of what has been studied in this field and what are the focuses of new research, in Brazil and in the world. Results showed that the topic agri-PV has experienced a considerable increase since the beginning of the 2020s, but there are still few studies published in Brazil concerning this topic in peer-reviewed scientific journals. Based on that, there is an important avenue of opportunities for future research evaluating the potential of Agri-PV systems on the Brazilian energy transition plan.

Keywords: agri-PV; land use hybridization; bibliometric research.

Introduction and Objectives: The growing global demand for food and energy drives changes in land use, which makes it desirable to increase agricultural and energy production with lower environmental impacts, in line with the sustainable development goals established by the United Nations.

In this context, agri-PV is a land use hybridization method that can increase land use efficiency, combining photovoltaic generation with productive uses such as agriculture, livestock and ecosystem services, among others. However, despite the desired increase in efficiency, in its current stage of technological development, agri-PV installations may incur in higher operation and installation costs and greater project complexity, which may hinder their adoption.

This theme has gained worldwide relevance mainly since the beginning of the 2020s and is relatively new in Brazil, requiring investments in research and development to address this strategic issue, and to understand the opportunities and limitations of this type of intensification of land use for the climatic conditions of Brazil. This work carries out a bibliometric evaluation on the agri-PV theme and seeks to present an overview of what has been studied in this field and what are the focuses of new research, in Brazil and in the world. The bibliometric search is one of the inputs that lay the foundation for the project "Agri-PV system: combining solar energy production with food production and climate change adaptation ("AgriPV_Brazil")", which intends to install an agri-PV system at the ESALQ campus in Piracicaba.

Methodology: The bibliometric research was restricted only to peer-reviewed scientific journals and carried out using the Scopus database. The logical sentence inputted to the "Search documents" field of the Scopus database to retrieve the papers information: "agrivoltaic*" OR "agri-voltaic*" OR "solar AND farming" OR "solar AND agriculture" OR "crop-solar AND systems" OR "photovoltaic* AND farming" OR "solar AND cropping" OR "solar-agri AND integration" OR "agro-solar AND hybrid" OR "crop-integrated AND solar" OR "farm-embedded AND solar" OR "agri-solar AND synergy" OR "solar-cultivation AND interface" OR "crop pv AND integration" OR "green AND energy AND agriculture" OR "solar AND agroecosystems" OR "agri pv" OR "dual AND use AND photovoltaics" OR "co-location AND photovoltaic*" OR "agri-solar" OR "solar AND sharing" OR "coexistence AND photovoltaic*" OR "agri-photovoltaics" OR "agrovoltaic*" OR "agro voltaic*". The search

engine was configured to search the aforementioned logical sentence within Article title, abstract and keywords. The software VOSviewer was used to process the data by sorting the papers by country and year of publication and by checking the co-occurrence of keywords that occurred at least five times.

Preliminary results: The research resulted in 238 documents, 90% of which were published after 2020. The main subjects that encompass those documents are energy, environmental science, engineering, agricultural and biological science. When comparing the publications by country our search found only 3 documents published in Brazil. From these three documents, two of them are related to animal thermal comfort and one was conducted in the cassava crop system in Colombia. Keyword network analysis showed five main clusters: i) solar power generation and agrivoltaics; ii) crops and photovoltaic system; iii) land use and agriculture; iv) climate change and food production; v) energy and sustainable development. Further when analyzing the keyword network by the year we can observe a change in the strength of the keywords from photovoltaic cells and photovoltaic system in 2020/21 to agrivoltaics and photovoltaics in 2022/23.

Preliminary conclusions: According to the results of the bibliometric research, agri-PV is a relatively new research topic which has experienced considerable relevance increase since the beginning of the 2020 decade. The bibliometric research also found little research in Brazil concerning this topic published in peer-reviewed scientific journals, which highlights the importance and relevance of this theme in the country. Regarding the keywords and subjects associated with agri-PV, the theme shows an intimate relation with energy transition and climate change, as shown by the bibliometric research, since it combines renewable energy and agriculture. The change in the strength of keywords from 2020/21 to 2022/23 suggests a shift towards the implementation of agri-PV systems in opposition to the suitability of specific solar cells for agri-PV systems.

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Abstract Title: Real time monitoring of submarine transmission systems in offshore applications

Authors' Names & Affiliation Institutions of all authors (in order for publication): José Roberto Cardoso (USP), Cássio Guimarães Lopes (USP), Eduardo Coelho Marques da Costa (USP), Mario Leite Pereira Filho (IPT), Rooney Ribeiro Albuquerque Coelho (USP), Ronaldo Francisco Ribeiro Pereira (UFAC), Andrei Oliveira Mota Porfiro (USP), Gabriel de Castro Biage (USP), Rafael Nascimento (USP).

Abstract: The emerging offshore systems require a continuous development of techniques applied to monitoring and reliability assessment, especially for electric power generation and transmission systems, as well as oil/gas prospection in deep water. Such applications demand a continuous monitoring and periodic evaluations of submarine cables, which are mostly inaccessible by visual inspection. For example, these power cables are usually applied to drive submarine motors with variable rotation velocity; power transmission from offshore wind farms to onshore substations; power delivery from land suppliers to oil/gas platforms; and several other specific facilities. In addition, several other indexes are needed for the accurate and reliable prediction of the dynamic loading capability of power transmission systems, in which the prior knowledge of the electrical parameters is crucial. In electric power transmission, the submarine cables are usually composed of three coaxial conductors and an external armor, which are characterized by self and mutual parameters: series resistance and inductance; transversal conductance and capacitance. Such electrical parameters are intrinsically related to the aging and degradation in which submarine cables are subject, as well as the propagation characteristics and maximum loading supported by the transmission system. Thus, it is possible to assess the cable health and reliability by means of the continuous monitoring of the loadability, as a function of the electrical parameter's variation in time. In this context, this research project proposes an efficient methodology for admittance and impedance parameters estimation, based on identification and optimum filtering techniques, from noisy current and voltage measurements at the sending and receiving ends of the submarine cable. By assuming an accessible and continuous measurement source, the cable parameters can be estimated periodically, and therefore important indexes on voltage stability and loadability can be mined from the submarine transmission system, such as: the surge impedance load – SIL, maximum power, and P-V stability margin. In this sense, the methodology premise lies on the periodic and continuous monitoring of parameters and stability margin, since both are intrinsically

related to the cable integrity in mechanical and electrical terms. Finally, the real time monitoring methodology will be evaluated by a rigorous procedure based on computational simulations and experimental results. Assuming that such validation process will produce a massive data set, it will be further used for evaluation on the feasibility of an additional methodology for prediction and classification of fault events, by using data mining, machine learning and clustering techniques.

Keywords: Offshore systems; Monitoring; Reliability assessment; Electric power generation; Transmission systems; Oil/gas prospection; Submarine cables.

Introduction and Objectives: The main objective of this research project is to develop a reliable and robust monitoring methodology for power transmission systems in offshore facilities, based on records and accessible measurements of current and voltage at the terminals of the submarine cable.
In order to achieve the main goal, the following specific objectives have been established: • Development of models which represent accurately the electric parameters and electromagnetic characteristic of submarine power cables, for transient and steady-state simulations; • Simulation of current and voltage measurements, obtained from transformers and Phase Measurement Units – PMUs, with proper noise modelling;
• Development of accurate and reliable estimation methods for electrical parameters and phasor estimation from noisy measurements;
• Assessment of the power-voltage stability (dynamic P-V profile) of power transmission systems based on the time-varying parameters estimation of submarine cables;
• Feasibility analysis on the aging/degradation prediction and monitoring of power cables based on the correlation between the electrical parameter's variation and voltage stability features; • Installing a laboratorial structure for experimental tests and validation of the proposed estimation and monitoring methodology;
• Validation of the proposed methodology by experimental tests for different conditions, e.g.: varying noise level in measurements, cable structure (mechanical and electrical characteristics), loading and power source;
• Determining a data base for evaluation on the feasibility of fault prediction and classification.

Methodology: The research project is structured into six stages, which also represent the execution methodology and activities. However, the principal division is given in terms of computational modelling/simulation activities and experimental tests. The former consists in the development of computational models of the submarine transmission system for current and voltage measurement simulations, and computational algorithms for parameters estimation/monitoring. As for the latter, a laboratorial infrastructure will be installed for experimental validation of the proposed estimation and monitoring methodology.
Most of the knowledge and methods to be applied for modelling, simulation, estimation, monitoring and experimental expertise have been produced by research groups of the LMAG – Laboratory of Applied Electromagnetism, Laboratory of Signal Processing, LGrid – Advanced Electric Grids Laboratory at the Polytechnic School and IPT – Institute of Technologic

Researches, at the University of São Paulo. These researchers compose the coordination and staff of the proposed project, in which the scientific and technological production is referred in the literature survey and bibliography of this project The activities are structured into the following six stages.

i. Cable modelling for computational simulations

ii. Development of the parameter estimation algorithm

iii. Transmission system monitoring from stability indexes and parameters.

iv. Laboratorial infrastructure and experimental analysis

v. Experimental data acquisition

vi. Feasibility analysis on a monitoring and prediction system

Preliminary results: At the present stage of our project, we do not have preliminary results to share, as the project has recently begun. However, we have outlined our anticipated expected results and deliverables, which we aim to achieve as the project progresses:

• Technical Reports covering submarine cable modelling and time domain simulations of current and voltage measurements at transmission terminals.

• Noise Modelling and Phasor Estimation as a theoretical introduction to noise modelling, simulation of noisy measurements, and an explanation of phasor estimation applied to noisy signals in the time domain.

• Parameter Estimation Method Development focusing on developing a method for estimating parameters. It includes validation across various load scenarios, noise levels, and sample sizes, along with an analysis of how cable electric parameters impact transmission system voltage stability. • Experimental tests and validation to improve the estimation/monitoring methodology, including a correlation analysis of estimated parameters with stability margin monitoring, comparing experimental and simulated data.

• Comprehensive documentation of the estimation/monitoring methodology and conclusions about its feasibility for predicting and diagnosing faults in submarine power transmission systems. • Dissemination of results and methodology through publication in reputable journals and presentations at relevant conferences, subject to TotalEnergy's consent.

• Technical knowledge and qualifications of team members in the field of power transmission systems for offshore applications.

Preliminary conclusions: While our project is still in its early stages, we do not yet have Preliminary findings or conclusions to share. This initial phase represents a crucial foundation upon which we will build our research journey. During this formative period, our focus has been on establishing a robust approach that will serve as the basis for our investigations. We have been diligently working to lay the groundwork for our project, which involves defining the scope, conducting a comprehensive literature review, and adjust our research objectives. This preparatory phase is essential to ensure that our subsequent efforts will be strategically aligned with the goals we aim to achieve.

Sergio Luciano Avila
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Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Wind turbine diagnostics based on current signatures: a review

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Abstract: Improvements in the operational monitoring of wind turbines are mandatory due to catastrophic accidents that have been occurring. The monitoring methodology most used by the industry uses mechanical vibration analysis. Another approach is to use the machine current signature analysis (MCSA) for condition monitoring. MCSA typically uses frequency domain analysis of the current signal through steady-state machine operation. An advantage of MCSA over other techniques is the simplicity of its instrumentation. There is no requirement for complex mechanical adjustments like the ones needed for vibration sensors (accelerometers and proximeters). Nevertheless, interference and noise severely hinder the MCSA. Monitoring both mechanical and electrical characteristics can provide a better understanding of time series analysis. This abstract presents a diagnostic exercise using mechanical vibration and current signature on a lightweight induction motor. Furthermore, we are developing a literature review of MCSA applied to wind turbines.

Keywords: wind turbines, current signatures, diagnostics, review.

Introduction and Objectives: This summary is the first result of the MitDev project. The motivation and objectives of the project are: the electrical variables of a wind turbine (typically voltage, current and power measurements) have characteristic frequencies that are orders of magnitude greater than the characteristic frequencies of variables related to mechanical components. These electrical variables are already measured to serve as input to the turbine control system. However, they are not all processed by the SCADA system nor sent to the central monitoring system because they constitute a volume of data that is too large for communication. These electrical signals are rich in harmonics and contain information that can anticipate electrical failures.

We will first understand the type of processing that must be done on electrical variables to detect deviations and anomalies. Subsequently, we must develop algorithms to carry out this processing in a robust and efficient way. Next, you will specify the hardware needed to do this

processing locally. Finally, we will be implementing and testing the system.

Methodology: For this abstract, first we presented a diagnostic exercise using mechanical vibration and current signature on a lightweight induction motor in laboratory. Afterwards, we are developing a literature review of MCSA applied to wind turbines.

Preliminary results: The accuracies presented by our methodology reach 100% for mechanical signals and about 95% for electric current for a lightweight induction motor in laboratory. It is noteworthy that we have been operating directly from raw data, requiring no feature extraction, such as frequency transformation. Moreover, using diverse data can be an advantage, like not having enough installation space for the vibration sensors or too noisy electric grids.

Preliminary conclusions: Just as relevant as a good understanding of the algorithm is to bring a laboratory application closer to the real-world issue. Noisy scenarios, kind, and severity fault classification (multiclass and nonlinear problem), and the required sample size by considering how accurate the classification result needs to be studied. Nevertheless, the literature using MCSA for wind turbines shows that the results are promising.

Thiago de Melo Augusto
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Abstract Title: SOFC – The future of Ethanol in the Transport sector

Authors' Names & Affiliation Institutions of all authors (in order for publication): University of São Paulo- Institute of Chemistry.

Abstract: Environmental impacts related to the increasing emission of greenhouse gases are a global problem, and decarbonization studies have garnered significant attention in scientific research. The development of technologies for decarbonizing the transportation sector, specifically using bioethanol and capable of replacing internal combustion engines with solid oxide fuel cells (SOFC) that produce H2 through internal reforming, is being investigated through various tools, including simulation, experimentation, and analysis. This project aims to develop Ni-based catalysts with low levels of noble metals (such as Ru, Rh, and Pd) by employing innovative strategies for nanoparticle synthesis and characterization, which will be assessed for ethanol reforming and subsequently capable of forming a layer to be deposited on the anode in fuel cells (SOFC).

Keywords: Solid oxide fuel cell; heterogeneous catalysts; ethanol steam reforming; hydrogen production.

Introduction and Objectives: One of the greatest challenges for global climate change is the decarbonization of the transportation sector. Transportation is responsible for 23% of global emissions and currently relies on hydrocarbons for 92% of its energy [1]. Portability is a key requirement for the energy source, which makes decarbonization of this sector difficult, as hydrocarbons are among the densest energy compounds available. On the other hand, vehicle emissions of pollutants such as particles, sulfur oxides, and nitrogen oxides are significant, necessitating cleaner sources of energy [1].

In this regard, efforts have been focused on batteries and polymer electrolyte fuel cells (PEFC) that operate with hydrogen, along with improvements in efficiency (e.g., hybrid vehicles) and fuel switching, such as the use of diesel or compressed natural gas instead of gasoline. Although batteries have been predominant over the last decade due to their advantages in manufacturing, cost, vehicle responsiveness, and infrastructure availability, fuel cells may offer long-term alternative advantages. Among these advantages, fuel cells have high energy density, whereas it is uncertain whether battery technology will ever advance enough to power long-distance transportation, such as ships or intercontinental flights. In applications like buses where fast charging or refueling is needed, fuel cells also have an inherent advantage. Finally, the broader advantage of transitioning to a hydrogen-powered transportation system is the production of the fuel itself, which provides a convenient option for storing intermittent renewable energy as a stable chemical product [2].

The field of catalysis has expertise in terms of tools and techniques for studying interfacial reactions at the atomic scale, as well as experience in surface modification to prevent or hinder undesirable reactions. These types of studies are necessary for the new materials that are under development, especially for the new protonic solid oxide fuel cells (SOFC), where a reliable set of complementary anodes and cathodic materials need to be developed, and issues of instability in high CO2 content atmospheres need to be resolved [3].

In this project, the goal is to develop Ni-based catalysts capable of performing ethanol reforming and hydrogen production, evaluated in conventional reactors and suitable for application in solid oxide fuel cells (SOFCs). An approach to improvements using dopants such as Ru, Rh, Pd, Pt, and Re, with the aim of minimizing parallel reactions and increasing hydrogen selectivity, is necessary. Consequently, the materials with the best performance can be used as layers on the anodes of solid oxide fuel cells.

Methodology: The catalysts will be electronically and structurally characterized using various techniques. Atomic absorption spectrophotometry (Shimadzu AA6300) will be conducted to evaluate the metallic composition of the materials. Thermogravimetric and CHN measurements will be performed in the Analytical Center (IQ-USP). X-ray diffraction will allow for the determination and quantification of crystalline phases, as well as estimating the crystallite size. The size and morphology of nanoparticles will be assessed by transmission electron microscopy at the Analytical Center (IQ-USP) or at the National Nanotechnology Laboratory (LNNano - Campinas, SP). Nitrogen physisorption measurements will also be conducted to determine the surface area and porosity of the materials. The assessment of the acid-base character of the materials can be done through temperature-programmed desorption of CO2 or isopropanol

decomposition using CatLab PCS equipment with mass spectrometry analysis (Hiden Analytical) or gas chromatography (Agilent). Degree of dispersion measurements may be performed through hydrogen chemisorption on the same equipment. Infrared spectroscopy using the Shimadzu IR-Prestige21 equipment available in our laboratory, with a diffuse reflectance reaction cell (IRDifuss-Pike Technologies) or a transmission reaction cell, will provide information about the catalyst surface as well as the formation of intermediates/spectators during the reaction.
Catalytic tests will be carried out in the gas phase under atmospheric pressure conditions in the CatLab equipment, in a fixed-bed reactor, which may undergo thermal treatments (25 - 1000°C) under H2O and ethanol atmospheres, in their respective proportions, under a continuous flow (controlled by flow meters). The effluent gas will be quantitatively analyzed by a mass spectrometer (Hiden Analytical) and/or a gas chromatograph coupled to a mass spectrometer (GC-MS Agilent). All catalyst activity calculations will be performed with the development and improvement of the analytical part for product separation, calibration, and quantification.

Preliminary results: The project is in its initial phase, with the assembly of the reaction setup and the synthesis of catalysts in progress. The first results will be presented at a later stage.

Preliminary conclusions: Advancements in catalysts are crucial to achieving the necessary gains in terms of solid oxide fuel cell (SOFC) efficiency for applications in the transportation sector. One approach that may achieve some success is related to changing the microstructure of the anode to optimize the quantity and location of nickel, for example, by impregnating this metal (or other metals or alloys) into an oxide. The addition of extra reforming catalysts, which can be incorporated into an impermeable layer above the electrode, helps reduce carbon deposition, improving internal reforming. In this context, it can be concluded that, at this stage of the project, the literature review has indicated the need to develop promoted catalysts containing nickel and other metals like rhenium, which will be supported on ceria and/or zirconia oxide for evaluating their catalytic activity in ethanol steam reforming.

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Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Python Tool for Cost and Loss Analysis in Offshore Energy Transmission

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Abstract: Climate change constitutes a profound global phenomenon, attracting substantial attention and compelling governmental and industrial entities to mitigate their contributions to its amplification. In this context, the ascendancy of renewable energy sources, particularly in offshore applications, has precipitated a critical examination of efficacious energy transmission methodologies. This paper endeavors to fortify offshore electrification initiatives in Brazil and substantiate global decarbonization endeavors through an empirical evaluation of the efficiency and cost-effectiveness of High Voltage Direct Current (HVDC), High Voltage Alternating Current (HVAC), and Low-Frequency Alternating Current (LFAC) technologies. This study underscores the salient import of streamlined offshore energy transmission protocols, emphasizing their pertinence in advancing sustainable electrification undertakings within the Brazilian context and their role in consonance with global decarbonization objectives, with specific reference to offshore wind energy and Floating Production Storage and Offloading (FPSO) platforms.

Keywords: LFAC; offshore; transformers; Low-Frequency; High Voltage; Direct Current; HVAC; HVDC; FPSO.

Introduction and Objectives: Climate change represents a preeminent global exigency, precipitating substantial scrutiny and inciting concerted endeavors by governmental and industrial stakeholders to ameliorate their involvement in its exacerbation. Against this backdrop, the burgeoning maturation of renewable energy resources, notably those domiciled in offshore environs, assumes primacy. It is imperative to subject energy transmission mechanisms to rigorous inquiry, especially within the offshore milieu. The exigency of amplifying offshore electrification schemes in the Brazilian theater, coupled with an earnest aspiration to undergird global decarbonization imperatives, impels a comprehensive analysis of three cardinal technologies: High Voltage Direct Current (HVDC), High Voltage Alternating Current (HVAC), and Low-Frequency Alternating Current (LFAC). This project accentuates the cardinality of proficient offshore energy transmission, with a punctilious accent on the wind energy offshore and Floating Production Storage and Offloading (FPSO) contexts. The primary aim of this empirical investigation is to operationalize cost functions and ohmic loss considerations pertaining to transmission equipment. The ultimate objective is to discern the optimally efficient offshore transmission solutions, with an emphatic focus on offshore wind energy generation and FPSO applications. The resultant findings hold potentiality for invigorating sustainable electrification paradigms within the Brazilian milieu and engendering synergies with the broader global decarbonization trajectory, thereby engendering a salubrious transformation of the energy matrix towards sustainability.

Methodology: The modus operandi germane to this research endeavour is anchored in the delineation of bespoke modules, each dedicated to the systematic evaluation of pertinent transmission equipment and associated factors endemic to offshore transmission analysis. These modules are configured to ingest rudimentary input parameters, encapsulated within a spreadsheet framework, and subsequently interrogate these parameters via a bespoke suite of Python-based functions. These functions, upon execution, yield robust estimates of transmission infrastructure costs concomitant with the concomitant technical losses. Subsequent to this quantitative scrutiny, the ensuing insights are expected to promulgate the identification and delineation of paragons of efficacious offshore energy transmission solutions. These findings, when amalgamated, are envisaged to engender a transformative infusion of sustainability within the broader energy matrix, commensurate with the exigencies of the global decarbonization agenda.

Preliminary results: Our initial analysis highlights a significant issue with existing mathematical cost models for offshore energy transmission. A substantial portion of these models is obsolete, ill-suited to account for the evolving landscape of offshore transmission technologies. Anticipations point toward substantial cost reductions in LFAC technology adoption. These reductions are expected due to the maturation and optimization of LFAC transformer production processes, which are foreseen to markedly decrease associated costs. An intriguing observation arises concerning the design and dimensions of LFAC offshore transformers. By manipulating transformer dimensions and emphasizing increased height over horizontal area, it becomes a viable strategy for positively impacting overall production costs. This design approach reduces iron consumption for the transformer core while slightly increasing the use of copper in the wiring. Given the cost-effectiveness and lighter weight of copper compared to iron, this design strategy holds promise in contexts with limited height restrictions.

Preliminary conclusions: The findings emphasize that the creation of new cost models, while important for providing an initial cost estimate, may not hold the same significance as other facets of research, such as transformer dimensions and weight. This perspective stems from the recognition that cost models would inevitably become outdated shortly after the technology's widespread implementation. Consequently, while an initial cost estimate might be feasible, it should be viewed as a temporary reference, and its relevance should diminish as the industry becomes more acquainted with LFAC technology.
The research underscores the transformative potential of LFAC technology in offshore energy transmission, particularly in contexts with height flexibility. The observed influence of transformer dimensions on production costs offers an intriguing avenue for cost optimization and resource utilization. Further empirical studies and practical implementations are essential

to validate and refine these insights, thereby advancing our understanding of the evolving landscape of offshore energy transmission technologies.

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Abstract Title: Processing of ceria-based oxides for use as electrolyte in a solid oxide fuel cell

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Abstract: Ceria oxide doped with gadolinium was prepared for use as an electrolyte in intermediate-temperature solid oxide fuel cells (SOFC). Ceramic powders of ceria doped with gadolinium (CGD) were processed by the solid-state reaction method. GDC powders were calcined at 1350 °C for 12 h. After confirming the crystalline phase, the powders were formed using a uniaxial and isostatic press in a cylindrical mold to obtain green samples in the form of tablets. The compacts were subjected to a densification process using the conventional sintering method, using a resistive furnace for a fixed time of 12 hours, varying the sintering temperature from 1400°C to 1550°C, with adopted heating and cooling rates of 5 °C per minute. The structural and morphological properties of the fractured surfaces of CGD ceramics were investigated by X-ray diffraction (XRD) and scanning electron microscopy (SEM), respectively. The XRD patterns obtained for all sintered samples confirm the presence of GDC phases and the absence of second phases. Finally, impedance spectroscopy measurements were carried out at various temperatures (from 200 °C to 700 °C) to evaluate the electrical properties.

Keywords: Ceria oxide based, SOFC, Electrolyte, Ionic conductors, Impedance spectroscopy.

Introduction and Objectives: The efficient use of SOFC technology is an important strategy for sustainable energy generation and climate change mitigation planning. However, there are challenges to the widespread commercialization of SOFCs, including the need to minimize their handling, reduce their cost, improve their performance, and adapt them to the use of alternative fuels to hydrogen, such as ethanol and biogas. An important strategy to minimize SOFC cost and increase cell durability is to reduce both processing and operating temperatures. For scale production of SOFC, it is necessary to develop low customized processing techniques for manufacturing multifunctional layered ceramic components with controlled microstructure and lowering the sintering temperature. Furthermore, the development of new materials and the use of advanced technologies are important to increase the efficiency of an SOFC operating at extreme temperatures. To achieve this, electrolytic materials with high ionic conductivity, electrodes with high occurrence activity, efficient studies, and a decrease in interfacial resistance between cell components are required for operation at extreme temperatures. Thus,

the general objective of this work was to carry out post-ceramic processing and then obtain ceramics based on ceria oxide for application in electrolytes in a solid oxide fuel cell. The objectives of the work were also to evaluate the physical properties through structural, microstructural and electrical characterizations.

Methodology: Gadolinium-doped ceria ceramic materials were initially obtained in the form of ceramic powders by the conventional method of mixing oxides or solid-state reactions. Once the gadolinium-doped ceria oxide (CGD) powders were identified with the desired phases, they were characterized morphologically and by thermal properties. After this step, the ceramic powders were shaped into discs (using a 15mm cylindrical steel mold) and cold compacted in a uniaxial press. Then, the ceramic discs were sintered using the conventional sintering method in a resistive furnace, with the synthesis conditions defined by a study carrying out dilatometry measurements. Finally, the characterization of the samples in the form of ceramic discs or specimens was investigated using the techniques of X-ray diffraction, RAMAN spectroscopy, scanning electron microscopy and impedance spectroscopy to evaluate the electrical properties.

Preliminary results: The Ce0.9Gd0.1O2 ceramic powders were processed by the state reaction method solid and presented a single crystalline phase identified with the type of fluorite structure for ceria oxide. According to literature data and confirmed by the study, the calcination temperature (heat treatment) used was 1350°C for 12 hours, with heating and cooling rates of 5°C per minute. With the ceramic powders characterized below, the (uniaxial pressing) in a cylindrical mold to obtain green samples. The compacts were subjected to a densification process by the conventional sintering method, using a resistive furnace for a fixed time of 12 hours, varying the sintering temperature from 1400°C to 1550°C, with adopted heating and cooling rates of 5°C per minute. The diffractograms of X-rays of all ceramic sintering conditions revealed the presence of peaks characteristic of the fluorite phase of the ceria oxide system. Furthermore, Raman spectra confirmed the presence of a single band characteristic of ceria doped with gadolinium, located at the position of 458 cm-1. Density measurements together with micrographs scanning electronics, demonstrated that ceramics have low porosity, indicating good densification, with a relative density greater than 95%, which is desirable to obtain excellent quality electrical measurements.

Preliminary conclusions: The ceramic powders of gadolinium-doped ceria were successfully obtained by the conventional method of oxide mixing or solid-state reaction and presented only a single phase. The morphology of the powders has a single average particle size distribution with a particle size of around 0.5 microns. The ceramics were sintered by the conventional sintering method or solid-state reaction and presented only one crystalline phase identified with the fluorite structure. Scanning electron micrographs of the ceramics revealed a microstructure with an average micrometric grain size and low porosity, corroborated by relative density measurements above 95%. Finally, the electrical measurements showed agreement with the literature results, being close to those reported for this composition of ceria doped with

gadolinium.

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Abstract Title: Algorithm for Fault location of onshore wind farm collector network based on artificial intelligence ("faultAIfinder")

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Abstract: Focused on fault location in onshore wind farm collector networks, the proposed research project aims to develop a hybrid system composed of intelligent diagnostics for faults (detection, classification, and localization) and aerial supervision using drones. The system is classified as hybrid because it combines various intelligent techniques for diagnosing faults with aerial supervision. The first step involves conducting a comprehensive literature review on the primary location techniques for distribution networks with overhead or underground lines (or both simultaneously). Afterward, an algorithm for fault location in aerial and/or underground distribution feeders will be developed for computational implementations with simulations.

Keywords: Fault Location, Artificial Intelligence, Onshore Wind Farm, Distribution System.

Introduction and Objectives: Several sections of onshore wind farms are prone to various types of faults, including short circuits. Locating faults in medium voltage feeders with both overhead and underground lines present a complex challenge due to factors such as the presence of distributed generation, extensive physical infrastructure, limited accessibility, and frequent alterations to these distribution lines. The research project's primary objective is to create an efficient and intelligent system capable of detecting, classifying, and pinpointing faults in medium voltage feeders within onshore wind farms, using aerial drones equipped with thermal

and high-resolution imaging capabilities. As an integral part of the hybrid system, the aerial support provided by drones will assist and provide essential information to the maintenance team concerning the overall fault location scenario and physical elements involved. This will result in reduced arrival and maintenance times, optimizing the repair process.

Methodology: Firstly, conducting a comprehensive literature review of methods used for fault location in distribution systems is crucial for defining the procedures and techniques that will be employed in developing the fault location algorithm. This review will be categorized into three primary fault location methods: intelligent algorithms, traveling wave analysis, and apparent impedance measurements. Each of these categories will be organized chronologically to provide a historical context for their development. To facilitate this review, we will primarily utilize reputable platforms such as IEEE Xplore, which hosts a vast collection of journals and papers relevant to our research project's area of interest. Subsequently, we will perform a comparative analysis of these location methods, with a specific focus on identifying their strengths and weaknesses. This analysis will serve as the foundation for the development of an intelligent algorithm capable of pinpointing faults. Building upon the insights gleaned from the literature review, our intelligent algorithm will be crafted to address existing gaps in the field and demonstrate its contribution in a meaningful way. The study aim to go beyond existing algorithms and provide innovative solutions to enhance fault location in distribution system.

Preliminary results: Currently, the primary phases linked to the project's progression pertain to three key areas: conducting a literature review concerning the test system selection, fault detection, classification, and localization, as well as the utilization of drones in overseeing electrical power systems. Consequently, the preliminary findings reflect the information gathered from relevant literature sources, particularly with regard to onshore wind farms and their relevance to the aforementioned project components. However, it's worth noting that there are as yet no definitive aspects to report.

Preliminary conclusions: The initial findings mirror the information extracted from relevant literature, with a specific emphasis fault location algorithms aplyed to wind farms systems. Unfortunately, no definitive aspects can be reported at this time

SHORT ORAL SESSION D

08/11 15h20 Short Oral Session D

0811 - NBS17 (TV1)

Chairs: Carlos Cerri – Maurício Cherubin

Bruna Emanuele Schiebelbein
Escola Superior de Agricultura Luiz de Queiroz - Universidade de São Paulo

Abstract Title: Status of soil health in agricultural soils in Brazil using the Soil Management Assessment Framework (SMAF)

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Abstract: Soil provides vital environmental services and plays a central role in achieving the Sustainable Development Goals. However, 40% of the world's soils are degraded, posing a challenge to food production. Soil health, an indicator of a soil's sustainable ecosystem functionality, is critical not only for crop productivity, but also to counter biotic and abiotic stressors. For example, healthier soils have been shown to produce higher yields and be less vulnerable to climate change. - The Soil Management Assessment Framework (SMAF) is one of the most advanced analytical models for assessing soil health. Therefore, the objectives of this work were i) to assess the health of Brazilian agricultural soils using the SMAF tool, and ii) to evaluate differences in soil health at the national scale, using a large set of agricultural data representative of Brazil. To calculate the Soil Health Index for agricultural areas in Brazil, a dataset of 23,997 sample points distributed in 15 Brazilian states and collected in 2021 and 2022 was used. These sample points were obtained from soybean agricultural areas. The SMAF was used to assess soil health at the national level using a minimum data set of five soil health indicators (P, K, pH, Bd and SOC), and the results of the soil health indicators were converted into a score ranging from 0 to 1 (unitless) using algorithms implemented in an Excel® spreadsheet. Finally, the scores for each indicator were integrated into an overall Soil Health Index (SHI) ranging from 0 to 1. The SHI and both indicator scores were interpolated using geostatistical techniques to create a map of spatial variation in soil health and to identify local

hotspots of soil health. Exploratory analyses and box plots were performed to evaluate the ISS and score indicators in different biomes and regions of Brazil. The results showed significant variation in soil health indicators among different Brazilian biomes. In general, the 0-10 cm soil layer is operating at more than 80% of its maximum potential, indicating opportunities to improve soil health through sustainable practices. The SMAF results highlight the inherent influence of climate and soil characteristics on soil health. These findings underscore Brazil's pivotal role in promoting soil health and advancing sustainable agricultural efforts globally.

Keywords: soil quality, soybean croplands, biomes.

Introduction and Objectives: Soil plays a critical role in providing environmental goods and ecosystem services essential for human well-being and achieving the Sustainable Development Goals. However, approximately 40% of the world's soils are degraded, posing one of the greatest challenges to food production. Maintaining and improving soil health is necessary to ensure food security and promote sustainable agricultural development. Globally, the concept of soil health is associated with the continued ability of soil, as a living ecosystem, to perform its functions related to maintaining environmental quality (air and water), promoting human health, and supporting crop productivity. In addition to ensuring crop productivity, healthy soils are critical to reducing crop vulnerability to biotic and abiotic stresses. For example, a recent study in China ((Qiao et al., 2022). found that crops (such as maize, wheat, and rice) grown in healthy soils had higher yields (10.3 ± 6.7%) and lower losses (up to 21%) due to reduced sensitivity to climate variability. Thus, the health of agricultural soils is directly linked to success in addressing major global challenges such as food security and climate change mitigation and adaptation. Due to its broad and complex nature, there is no direct way to measure soil health. Instead, its assessment relies on the integration of chemical, physical, and biological indicators and their interactions. These indicators provide insight into overall soil health, help monitor changes over time, and differentiate between different management practices. With growing global interest and the potential to achieve sustainable development goals through healthy soils, computational approaches have been developed, such as the Soil Management Assessment Framework - SMAF, which is one of the most advanced analytical models. The assessment involves three steps: i) selection of a minimum data set, ii) interpretation of the evaluated indicators, and iii) integration of the indicators into an overall index. In Brazil, several local studies have evaluated soil health using the SMAF tool, highlighting its applicability and sensitivity in distinguishing agricultural crop diversification and land use in the Central South region of Brazil, effects of sugarcane straw removal, agroforestry systems, mangroves, and technosols. Therefore, the objectives of this work were i) to assess the health of Brazilian agricultural soils using the SMAF tool, and ii) to Evaluate differences in soil health at the national scale, using a large set of agricultural data representative of Brazil.

Methodology: To calculate the Soil Health Index for agricultural areas in Brazil, a dataset of 23,997 sample points distributed in 15 Brazilian states and collected in 2021 and 2022 was

used. These sample points were obtained from soybean agricultural areas, which include major grain-producing regions. The data were obtained from a large national initiative led by Bayer S.A. in collaboration with public research institutions, including ESALQ/USP. The SMAF was used to assess soil health on a national scale using a minimum data set of five soil health indicators. The chemical indicators included pH, related to soil acidity, and K and P, related to nutrient cycling, which are key drivers of plant growth and productivity. Bulk density (Bd) served as a physical indicator of soil processes such as aeration, water dynamics, and mechanical resistance to root growth. In addition, soil organic carbon (SOC) was considered a driver of multiple processes and functions, such as nutrient cycling, maintenance of soil structure, and carbon sequestration. These indicators have been widely used in soil health studies both in Brazil and globally. In the second step, the results of the soil health indicators were converted into a score ranging from 0 to 1 (unitless) using algorithms implemented in an Excel® spreadsheet. These scoring curves were specific to each soil type, soil texture, mineralogy, climate, sampling season, slope, crop, and analytical method. In the third and final step, the scores for each indicator were integrated into an overall Soil Health Index (SHI) ranging from 0 to 1 (Equation 1). This value represented the percentage of the total potential functioning of the soil in terms of its ability to perform functions related to crop productivity, nutrient cycling, and environmental protection. SHI has been calculated for 0-10 cm soil depth.

$$SHI = \Sigma Score_i \times Weight_i$$

Where Scorei was the score of the indicator and Weighti was the weighted value of the indicators. The indicators were weighted based on the chemical components (pH, P, and K), physical components (Bd), and biological components (SOC). Thus, regardless of the number of indicators, each group had the same weight (33.33%) in the final index.

The SHI and both indicator scores were interpolated using geostatistical techniques to create a map of spatial variation in soil health and to identify local hotspots of soil health.

Preliminary results: Regarding the scores of the chemical indicators, both P and K show similar trends. Scores close to 1 are observed in the Pampa (P: 0.99; K: 0.94) and Atlantic Forest (P: 0.98; K: 0.94) biomes. In contrast, the Cerrado (P: 0.97; K: 0.86) and Amazon (P: 0.97; K: 0.79) biomes recorded lower scores, especially for K. Regarding pH, scores close to 1 were found in the Cerrado (0.93) and Atlantic Forest (0.92) biomes, while the Pampa and Amazon biomes recorded lower values, with values of 0.85 and 0.89, respectively. For soil density, the Pampa had the highest value (0.82), while the Atlantic Forest, Amazon, and Cerrado had lower values of 0.76, 0.76, and 0.73, respectively. For SOC in general, all biomes had scores close to 1 (Pampa -0.98; Atlantic Forest -0.96; Cerrado -0.95; and Amazon -0.88). Finally, in terms of ISS, the Pampa (0.90) and Atlantic Forest (0.88) biomes had the highest ISS scores, compared to Cerrado (0.86) and Amazon (0.83). These results correlate with climatic variables such as temperature and precipitation. The humid subtropical climate (Cfa and Cfb) regulates soil carbon accumulation by slowing the rate of organic matter decomposition and promoting greater plant biomass production. Meanwhile, the presence of highly weathered soils with

natural fertility suggests specialized carbon sequestration mechanisms that further enhance carbon storage potential and improve nutrient availability for plants.

Preliminary conclusions: Overall, the 0-10 cm soil layer is operating at over 80% of its maximum capacity across the biomes studied. This suggests that there's still potential to further improve soil health through sustainable management practices. The SMAF tool has proven effective in assessing variation in agricultural soil health in Brazil. However, there's room to refine its interpretation curves by incorporating different soil classes and the diverse climatic conditions found throughout Brazil, which could yield even more accurate results. These results underscore the influence of climate and soil characteristics on SHI and highlight Brazil's unique ability to play a central role in promoting soil health and advancing sustainable agricultural practices on a global scale.

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Esalq/ USP

Abstract Title: Nature-based solutions: Sustainable development of Latin America

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Abstract: Latin America is a region with abundant natural resources and diverse cultures, much of which lies between the tropics. Sustainable agriculture and forestry practices can have a reduced environmental impact in this region compared to other parts of the world. These practices can create a balanced use of chemical inputs, harmonious relations between humans and soil-plants-livestock, and even provide a nature-based solution to climate change by sequestering carbon emissions. This paper presents condensed information from primary and secondary sources, representing established knowledge in the field of soil carbon sequestration in agricultural lands and its role in carbon neutrality. By implementing these strategies, we can support farmers while contributing to the objectives set by the Paris Agreement and the UN's Sustainable Development Goals.

Keywords: Nature-based solutions; Carbon sink in agricultural lands; Integrated agricultural systems, Living soils.

Introduction and Objectives: Latin America boasts abundant natural resources and a multitude of cultures. Thanks to its tropical location, the region benefits from more sustainable agricultural and pasture practices compared to other areas of the world. Therefore the region can spearhead the swift to the sustainable circular bioeconomy (Giampietro 2019; Keswani

2020) and, in doing so, contribute to tackling the deadliest market failure of our time: climate change (Chichilnisky et al. 2020).

Sustainable agriculture and forestry must take a central role in promoting sustainable resource use, while ensuring balanced chemical inputs and harmonious human-soil-plant relations.s (Zylbersztajn et al. 2021). This integration can bring, at the same time: better environmental management, nutritious food and feed, renewable energy and fibers, rich soils, and all these accumulated with viable ways to create income specifically to maintain the livelihoods of the communities around the natural resources. Soils represent a significant carbon (C) sink (as we will detail ahead), and the plants over it as well because they use carbon dioxide (CO2) in their photosynthesis process. Besides that, a considerable amount of 22% (IPCC 2022) of the global emissions is because of land use, land-use change, and forestry (LULUCF), reported by the Intergovernmental Panel on Climate Change, merged into a two-part volume referred to as Agriculture, Forestry and Other Land Use (AFOLU). This shows that the way we practice agriculture, pasture, and forestry is not sustainable and will not support the growing demand for food, feed, fiber, and energy in the future. Monoculture highly irrigated and chemically kept practices have caused soil degradation, reduced the area with natural cover, and also many forms of greenhouse gasses (GHG) emissions. This can be changed.

The American continent has a diverse surface cover, from forests, grasslands, deserts, savannahs, to fertile soil to agriculture. In terms of agricultural lands, pastures occupy the largest area (905 million ha), followed by croplands (340 million ha). In agriculture, the main area cultivated with annual crops is soybean (91 million ha), corn (72 million ha), and wheat (35 million ha). With a much lower area, sugarcane (14 million) and coffee (5 million ha) are the main semi-perennial and perennial crops, respectively, cultivated in the continent (Cerri et al., 2021). The complex matrix of soil, climate, vegetation, and management found across the continent maintains great variability of soil C stocks. The continental average soil C stocks for 0-30 cm were estimated at 51 Mg ha-1, ranging from 63 Mg ha-1 in Central America to 48 Mg ha-1 in South America (Cerri et al., 2021).

Methodology: This paper is a literature review, bringing together information from primary and secondary sources that the same authors of this paper prepared in many other technical documents and reports over the last five years. As such, it consists of a collection of established knowledge in the particular field of soil C sequestration in agricultural lands (soil, pasture, and crops) and its role in carbon neutrality as strategies that can be applied on large scales in Latin America, where the agriculture production is one of the main causes of national emissions of green gases to the atmosphere.

Furthermore, it identifies that the techniques available and technologies are at potentially low cost, being beneficial to farmers and, at the same time, contributing towards the goals set in the Paris Agreement. It intends to contain technical information about nature-based solutions in an easy and accessible format to readers from outside the area of soil C sequestration.

Preliminary results: The key point to this new economic paradigm is to develop effective and viable ways to sequestrate C. Sustainable farming is one of the best options available to that.

This was the conclusion of the report that the Inter-American Institute for Cooperation on Agriculture (IICA) created under the initiative Living Soils in the Americas (LiSAm, 2021), which is an extensive network involving governments, international organizations, universities, the private sector, and civil society organizations to join efforts against land degradation promoting soil health, C sequestration and other associated benefits to people and the environment. Limiting global warming to acceptable levels is not necessary to reduce GHG emissions but also to increase C removal from the atmosphere. While GHG emission reduction can be achieved by multiple sectors (energy, industry, agriculture, etc.), C removals are predominantly done by nature-based solutions, including agriculture and forests (Friedlingstein et al., 2020). In this context, Bossio et al. (2020) estimated that soil C represents about ¼ of NBS potential for C sequestration. No matter if more simplified or detailed, the "gold" principles to assess if a sustainable management practice is efficient in achieving soil sequestration are: 1) does it provides abundant and continuous C inputs into the soil that leads to an increase in C stocks; and at the same time 2) does it reduce GHG emissions that were coming from the soil, therefore reducing the C losses? These questions are important because not all the CO2 removed from the atmosphere by plants remains stored in the plant's biomass or in the soil for much time. Most of it, around 60-90% of the C that was incorporated as organic components, returns to the atmosphere when plants die or are harvested, and the rest of the biomass emits through the decomposition process (Cerri et al. 2021).
Four scenarios are particularly relevant to implementing these SSM: 1) in places where soil C stocks have reached equilibrium, there is the possibility to increase C levels through SSM; 2) where the soil C stocks are increasing slowly and could increase much more if SSM were adopted; 3) where soil C stocks shows signs of declining, and it is possible to stop or mitigate C losses with SSM; and 4) where soil C stocks are declining, but reversing this fall is possible through SSM (FAO 2020).

Preliminary conclusions:

The more diverse and integrated agriculture with forestry and pasture, the greater the possibilities to increase the provision of ecosystem services, among which is the ability of the living soil and plants to sink C from the atmosphere back into the ground. Another point is that the high amount of depleted soil needs to be recovered and the native vegetation restored to reduce emissions and to increase other ecosystem services that are fundamental to Latin America's mitigation, adaptation, and resilience to climate change. This strategy of ecosystem-based adaptation harnesses the increase in biodiversity and the indirect benefits of more ecosystem services that conservation, sustainable management, and restoration bring and are one of the most cost-effective to adapt and build the resilience of human communities and societies to the impacts of climate change (FEBA et al. 2022). Integrated agricultural systems and restored areas of native vegetation under SSM can secure productivity, increase soil C sequestration, increase food and energy production (Figure 7), as well as to protect water resources and fisheries; promote human health and wellbeing; strengthen people's livelihoods, build more equitable societies; rebuild and strengthen nature, and on top of all that reduce climate risks. Therefore, adopting NBS is essential to cool our planet and sustain vital resources

and living conditions (Girardin et al. 2021). If applied in the Americas, sustainable management practices will promote the SDGs and, at the same time, reduce climate change risks.
Therefore, new protocols for promoting soil health and soil C sequestration through curbing land degradation in the Americas can increase productivity, reduce environmental depletion, and create sustainable income for local businesses. Many are opportunities for Latin America to gain from NBS, but to achieve that, policies and markets need to be redesigned to place nature and people at the center of the economy. Organizations also need to transform themselves and commit to ESG so that business plays a transformative role in the economic transition. Banks and asset management recognize environmental and social risks to the company they finance, demand disclosure of ESG data and finance only nature-positive projects to accelerate the transformation.
Latin American countries can be protagonists in the climate agenda. Still, indeed, more empirical research is needed to increase the knowledge of the particularities of the region and, at the same time, create MRV protocols that can improve the regional consistency of data that is necessary for C credit integrity, and in doing so unlock new forms of NBS financing. A regional approach could potentially help implement improved practices at scale and benefit a greater diversity of farms by enabling access to and participation in markets.

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Abstract Title: Spectral signature of synthetic Fe-rich nanoparticle in an agricultural soil

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Abstract: The spectral signature can infer numerous soil attributes, such as the availability of elements, minerals, organic material, water, and physical properties. The alteration of these materials can directly influence the various ecosystem functions of the soil. Moreover, the use of synthetic nanoparticles in agricultural areas is also related to changes in soil properties, such as water absorption, nutrient availability, and acidity regulation. In this context, this study aimed to analyse the spectral signature of a synthetic Ferich nanoparticle and investigate the effect of its addition by comparing the absorption bands in regions influenced by organic C,

organic material, and molecular vibrations. The studied soil has sandstone origin from the Adamantina formation and was collected at the Study Farm of the School of Agricultural and Veterinary Sciences, UNESP, Jaboticabal, SP, Brazil. The synthetic Fe-rich nanoparticle was synthesized by the Laboratory of Catalysis of USP via hydrothermal means. Spectral analysis was performed on the synthetic nanoparticle in the soil and the combination between soil and nanoparticle after 30 days of reaction. Approximately 1 g of soil (air-dried earth) was ground in an agate mortar until constant colour was obtained and the content was placed in a sample holder with a cylindrical space of 16 mm in diameter to obtain diffuse reflectance spectra. Reflectance values were determined using a Lambda 950 UV/Vis/NIR spectrophotometer coupled to a 150-mm diameter integrating sphere. Spectra were recorded at 1 nm intervals, with an integration time of 2.43 nm s−1 over the range of 250 to 2,500 nm (visible).The synthetic nanoparticle absorbs little and has high reflectance, as it is a white material. The tested soil has sandstone origin and, therefore, presents higher reflectance due to the presence of lighter minerals, such as quartz, which absorbs less and reflects more. We observed a decrease in the spectral curves when the nanoparticle was added to the soil. While the nanoparticle alone has high reflectance, its combination with the soil reduces the natural reflectance. The synthetic nanoparticle shows several regions with influences of organic C, organic material, and molecular vibrations referring to water molecules and OH groups of minerals, as well as in the soil. The increase in intensity in bands relating to organic C or organic matter may indicate an improvement in soil fertility, such as an increase in cation exchange capacity. The combination of soil and the synthetic nanoparticle also caused a change in the intensity of bands that are characteristic of the minerals present in the soil. More detailed studies have been conducted to demonstrate the changes in crystalline structures and/or the quantity of minerals affected after the synthetic nanoparticle addition, as well as the benefits in ecosystem functions that this addition can promote.

Keywords: reflectance, soil minerals, synthetic nanoparticle.

Introduction and Objectives: The spectral signature can infer numerous soil attributes, such as the availability of elements, minerals, organic material, water, and physical properties. The general decrease in the spectral curve may indicate an increase in the proportion of dark minerals and/or organic materials and, therefore, absorb more light. The alteration of these materials can directly influence the various ecosystem functions of the soil. Moreover, the use of synthetic nanoparticles in agricultural areas is also related to changes in soil properties, such as water absorption, nutrient availability, and acidity regulation. In this context, this study aimed to analyse the spectral signature of a synthetic Fe-rich nanoparticle and investigate the effect of its addition by comparing the absorption bands in regions influenced by organic C, organic material, and molecular vibrations.

Methodology: The studied soil has sandstone origin from the Adamantina formation and was collected at the Study Farm of the School of Agricultural and Veterinary Sciences, UNESP,

Jaboticabal, SP, Brazil. The synthetic Fe-rich nanoparticle was synthesized by the Laboratory of Catalysis of USP via hydrothermal means. Spectral analysis was performed on the synthetic nanoparticle in the soil and the combination between soil and nanoparticle after 30 days of reaction.

Approximately 1 g of soil (air-dried earth) was ground in an agate mortar until constant color was obtained and the content was placed in a sample holder with a cylindrical space of 16 mm in diameter to obtain diffuse reflectance spectra. Reflectance values were determined using a Lambda 950 UV/Vis/NIR spectrophotometer coupled to a 150-mm diameter integrating sphere. Spectra were recorded at 1 nm intervals, with an integration time of 2.43 nm s−1 over the range of 250 to 2,500 nm (visible).

Preliminary results: The synthetic nanoparticle absorbs little and has high reflectance, as it is a white material. The tested soil has sandstone origin and, therefore, presents higher reflectance due to the presence of lighter minerals, such as quartz, which absorbs less and reflects more. We observed a decrease in the spectral curves when the nanoparticle was added to the soil. While the nanoparticle alone has high reflectance, its combination with the soil reduces the natural reflectance.

The synthetic nanoparticle shows several regions with influences of organic C, organic material, and molecular vibrations referring to water molecules and OH groups of minerals, as well as in the soil. These results show that the analysis allows the nanoparticle to be characterized using a spectral technique and verify the changes it can cause in the soil. The increase in intensity in bands relating to organic C or organic matter may indicate an improvement in soil fertility, such as an increase in cation exchange capacity.

The combination of soil and the synthetic nanoparticle also caused a change in the intensity of bands that are characteristic of the minerals present in the soil. More detailed studies have been conducted to demonstrate the changes in crystalline structures and/or the quantity of minerals affected after the synthetic nanoparticle addition, as well as the benefits in ecosystem functions that this addition can promote.

Preliminary conclusions: The results obtained so far indicate that the addition of nanoparticles to agricultural soils changes their spectral signature, which may influence some of their ecosystem functions in the future. However, we emphasize that more detailed and robust analyses have been conducted based on spectral signatures to identify which soil attributes are changing and the implications of these changes on their ecosystem functions.

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Abstract Title: Integrated crop-livestock systems and well-managed pasture promote biological activity, aggregates stability and the increase of soil organic carbon in southern Amazon, Brazil

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Abstract: Integration crop-livestock (ICL) systems are known to have higher diversity of roots and crop residues that favor microbial activity and increase the potential of soil carbon (C) sequestration. This study aimed to investigate the impact of different integrated agricultural systems on microbial indicators, total C content and aggregation over eleven-year period. A field experiment was conducted in a randomized block design with four replications and four treatments: Crop succession (CS) - annual production of soybean (Glycine max L.) followed by corn (Zea mays); Integrated crop-livestock system (ICL) - a rotation system of four years with soybean/corn production in the first year, soybean/corn + braquiaria (Brachiaria brizantha cv. Marandu) in the second year, and followed by two years of pasture associated with cattle production; Pasture (P) – continuous cultivation of Brachiaria brizantha (cv. Marandu) with cattle production; and Integrated crop-livestock-forest system (ICLF) – similar to ICL system, with the eucalyptus as additional forest component. Soil samples were collected to a 0.3 m depth, in which the total C, total nitrogen (N) contents, microbial biomass carbon (MBC), glomalin, enzymatic activities of β glucosidase, acid phosphatase and arylsulfatase were measured. In addition, the soil structural quality was measured from the mean weight diameter (MWD) of aggregates. Our findings revealed that P and ICL increased C (28%) at 0.1 m and N content at 0.05 m depths, while MBC was higher (50%) in all layers evaluated as compared to CS, thus indicating that MBC is more sensitive to management change relative to C content. Similar results were found for enzyme activity, especially at 0.05 m layer for all enzymes.

Regression analyses proved that C accrual was triggered by the increase in enzyme activity, due to the role of C as energy source for the microbiota. We found lower C/N ratio under ICL, and higher microbial quotient (qmic) under ICL and P, suggesting a better C utilization by the microorganisms. MWD and glomalin increased under P, ICL and ICLF at 0.1 m, indicating higher soil aggregation in these systems. Our study suggests that ICL and P systems play an important role in C accumulation by favoring microbial activity and soil aggregation when compared to more conventional cropping systems.

Keywords: Soil organic matter; Soil carbon stabilization; Soil microbiology; Soil enzymes; Soil aggregation; Soil health.

Introduction and Objectives: Integration crop-livestock (ICL) systems are known to have higher diversity of roots and crop residues that favour microbial activity and increase the potential of soil carbon (C) sequestration. This study aimed to investigate the impact of different integrated agricultural systems on microbial indicators, total C content and aggregation over eleven-year period.

Methodology: A field experiment was conducted in a randomized block design with four replications and four treatments: Crop succession (CS) - annual production of soybean (Glycine max L.) followed by corn (Zea mays); Integrated crop-livestock system (ICL) - a rotation system of four years with soybean/corn production in the first year, soybean/corn + braquiaria (Brachiaria brizantha cv. Marandu) in the second year, and followed by two years of pasture associated with cattle production; Pasture (P) – continuous cultivation of Brachiaria brizantha (cv. Marandu) with cattle production; and Integrated crop-livestock forest system (ICLF) – similar to ICL system, with the eucalyptus as additional forest component. Soil samples were collected to a 0.3 m depth, in which the total C, total nitrogen (N) contents, microbial biomass carbon (MBC), glomalin, enzymatic activities of β-glucosidase, acid phosphatase and arylsulfatase were measured. In addition, the soil structural quality was measured from the mean weight diameter (MWD) of aggregates.

Preliminary results: Our findings revealed that P and ICL increased C (28%) at 0.1 m and N content at 0.05 m depths, while MBC was higher (50%) in all layers evaluated as compared to CS, thus indicating that MBC is more sensitive to management change relative to C content. Similar results were found for enzyme activity, especially at 0.05 m layer for all enzymes. Regression analyses proved that C accrual was triggered by the increase in enzyme activity, due to the role of C as energy source for the microbiota. We found lower C/N ratio under ICL, and higher microbial quotient (qmic) under ICL and P, suggesting a better C utilization by the microorganisms. MWD and glomalin increased under P, ICL and ICLF at 0.1 m, indicating higher soil aggregation in these systems.

Preliminary conclusions: Our study suggests that ICL and P systems play an important role in C accumulation by favouring microbial activity and soil aggregation when compared to more

conventional cropping systems.

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Abstract Title: Deforestation Patterns Evolution of the Amazon Basin from 1985 to 2021

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Abstract: This study explores deforestation indicators in the Brazilian Amazon rainforest. Employing image processing techniques, we identified deforested patches over 37 years, spanning 3 million km2. Geometric measures assessed patch regularity and area, revealing clear trends: compactness followed a lognormal distribution, while equivalent radii decreased logarithmically. Cluster analysis was applied to group regions
with similar deforestation patches. The results were consistent with the east-to-west deforestation shift and each cluster displayed unique compactness and equivalent radii. The increase in the compactness time series indicates more organized
patches consistent with human-made deforesting. Equivalent radii distribution revealed patch enlargement within 1-2 km. These observed trends in compactness and
equivalent radii can be used in models studying the links between land use and climate change. They can also enhance understanding of Amazon deforestation, guiding evidence-based policies for its conservation.

Keywords: Land Use; Amazon Rainforest; Landscape Ecology; Fragmentation.

Introduction and Objectives: This study aims to analyse and describe deforestation patterns in the Amazon rainforest and how they have evolved. The land use patterns were classified based on their shape, size, and rate of deforestation, dividing the Amazon rainforest into four distinct regions, each with its unique characteristics. Unlike previous works on deforestation in the Amazon rainforest, which only studied small areas or limited periods (his study covers 36 years and an area of approximately
3 × 10^6 sqkm within the Brazilian Amazon.

Methodology: We used land use and land cover (LULC) maps from the MapBiomas platform. First we separated natural formations from those altered by human interference (e.g. pastures, cultures, mining etc). The images were processed and segmented, and each deforestation patch

was uniquely identified. These patches were characterized geometrically, calculating their compactness (a dimensional quantity defined as the ratio of the area and squared perimeter), equivalent deforestation radius and yearly deforesting rate. Using k-means aggregation, we identified four distinct regions in the Amazon rainforest (A to D), each with unique characteristics regarding the aforementioned geometric quantities.

Preliminary results: Starting from the more preserved region (easternmost) and going to the west (known as the "arc of deforestation"), we observed that compactness distribution values steadily grow until reaching a peak in the middle regions and receding at the westernmost region. The equivalent radii distribution is strongly peaked to the right, indicating that most deforestation patches' radii are under 2 km (approximately 12.6 sqkm). Analysing the time evolution of compactness with respect to the base year (1985) we realize that the compactness tends to increase. Increasing compactness indicates an area with smooth and regular edges, which is evidence of systematic human intervention substituting the forest for pasture and agriculture.

Preliminary conclusions: This study's use of equivalent radius and compactness as indicators has revealed intriguing characteristics that warrant further investigation. Notably, the highest values of compactness distributions are not observed within the most deforested region (D); rather, they emerge within the transitional zone between the eastern and western parts of the Amazon. This intriguing pattern raises the possibility of a critical threshold or 'tipping point.' The evolution of compactness also offers an opportunity for modelling to predict how these deforesting patches evolve and use these predictions in models that integrate the interactions between land use change and the emission of greenhouse gases.

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Abstract Title: Potential of Hydrogen Production in A Microbial Electrolysis Cell from Sugarcane Vinnasse

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Abstract: Currently, technologies for hydrogen production are widely studied due to be a zero-carbon energy at the point of end use. Among these, the bioelectrochemical process call the attention since they use microorganism as biocatalyzers. On the other hand, vinasse coming from ethanol production can be used as raw material for energy production in biotechnological

process due to the high concentration of organic matter. Therefore, the present research aim to evaluate the potential hydrogen production from vinasse by a recent bioelectrochemical process, better known as microbial electrolysis cell. Preliminary results in MEC with synthetic vinasse have indicated a production of at least 0.5 µmol of hydrogen per gram of organic matter removed.

Keywords: Hydrogen production; energy recover; microbial electrolysis cell; renewable energy.

Introduction and Objectives: Bioelectrochemical systems (BES) are a recent technology based on the capacity of some microorganisms for transferring or taking electrons toward or from a solid electrode. That is, BES is based on the development of biocatalyzers, where microorganisms are able to transform the chemical energy contained in the organic matter directly into electricity or hydrogen. These BES are better known as microbial fuel cell (MFC) and microbial electrolysis cell (MEC), respectively. In MEC, exoelectrogenic bacteria catabolize the substrate by using the electrode (anode) as terminal electron acceptor, and in the absence of oxygen, the addition of supplementary voltage drives the hydrogen evolution at the cathode. On the other hand, the economic growth of Brazil is largely supported by bioethanol production, which is a biofuel obtained from a renewable material, and its combustion is less aggressive for the environment, as compared to fossil fuels. However, each litter of bioethanol generates between 10 and 18 L of vinasse, which contains high concentration of organic matter, as well as antibacterial and recalcitrant compounds. However, this composition has become the vinasse in an interesting raw material for biotechnological processes for recovering energy and high value-added products. Therefore, this research project aims to assess the potential of a microbial electrolysis cell for hydrogen production from vinasse.

Methodology: For experimentation, two MEC of double chambers with activated carbon as support material for the biocatalyst formation is carried out under potential of 0.6 and 0.8 V. MEC were configured to two electrodes and the potential was supplied by a power supply Synthetic vinasse of 5 g COD/L is used as substrate and microorganisms are from a microbial fuel cell.

Preliminary results: MEC has produced biogas composed mainly of H2 and CO2 during inoculation and the enrichment of electrogens microorganisms. Traces of methane were observed at the beginning of the operation, with progressive decrease likely due to the application of potential. The initial hydrogen yield was 0.77 and 0.55 µmol H2 / g COD removed with potential of 0.8 and 0.6 V, respectively. Around 95% of organic matter contented in the synthetic vinasse was degraded.

Preliminary conclusions: Initial experiments indicated hydrogen can be produced in MEC from vinasse and the activated carbon has shown to be able for the biofilm formation.

Victória Santos Souza
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Abstract Title: Nature based solution: cover crops in the Cerrado and their role in greenhouse gas emissions and soil carbon distribution

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Abstract: Concerns about soil degradation and increasing atmospheric levels of greenhouse gases (GHG) (CO2, N2O and CH4) have stimulated interest in the potential of soil to mitigate climate change over the past few decades. The aim was to evaluate biomass production, soil C distribution and greenhouse gas emissions in a long-term (10 years) cover crop management system in the Cerrado. GHG emissions were analyzed during the soybean cycle on the biomass of cover crops in Rondonópolis – MT. The cover crops were: 1) Fallow; 2) Crotalaria spectabilis; 3) Urochloa ruziziensis; 4) U. brizantha (2 years) and maize/U. ruziziensis (7 years); 5) Cajanus cajan (2 years), Helianthus annuus/U. ruziziensis (3 years) and mix (C. spectabilis; P. glaucum; U.ruziziensis e C. cajan) (4 years). GHG fluxes were measured using manual static chambers. Four replicates were performed for each treatment. To determine the total weight of biomass in the sampled area, the cover crops were cut close to the ground and the entire biomass of 1 m² was collected. Physical fractionation of SOM was performed (Cambardella and Elliott, 1992). The soybean/U.ruziziensis showed the highest biomass production, higher C contents (g C/kg soil) in the MOP and MOAM fractions, and a soil sink for CH4. in addition to negative N2O fluxes through C. spectabilis. This assessment is essential for the calculation of the carbon balance of agricultural systems and for the definition of more promising management options for the mitigation of climate change. The data presented in this study are partial and refer to the year 2023/1, the study is ongoing and is expected to be completed in 2024/2.

Keywords: Cover crop mix; biomass; particulate organic matter.

Introduction and Objectives: Concerns about soil degradation and increasing atmospheric levels of greenhouse gases (GHG) (CO2, N2O and CH4) have stimulated interest in the potential of soil to mitigate climate change over the past few decades. Globally, about 75% of GHG emissions are derived from the energy sector, and from the burning of fossil fuels (OWD, 2020). In Brazil, the emission pattern differs from that observed globally, as 46% (998 MtCO2e) of emissions come from land use, 27% (577 MtCO2e) from the agricultural sector and only about 23% (494 MtCO2e) from the sectors energy and industrial processes (Potenza et al., 2021).
The main regions responsible for the increase in greenhouse gas emissions are the North (755 MtCO2e) and the Center West (446 MtCO2e) with 90% of the emissions (Potenza et al., 2021). These emissions are mainly due to the change of areas from forest to pasture (Potenza et al.,

2021). The states with the highest CO2e emissions are the states of Mato Grosso (85.3 MtCO2e) and Goiás (58.6 MtCO2e) which are important agricultural production regions in Brazil, with 71.488.025 Mt of soy produced in Mato Grosso and 23.185.268 Mt in Goiás (CONAB, 2022). Thus, the concern with the increase in GHG emissions has motivated the identification of efficient management and cultivation systems to generate a positive carbon balance, i.e., the sum of CO2 removal and storage in soil is higher than the sum of GHG emissions in a given period of time.

In this sense, the adoption of management practices that reduce GHG emissions and increase C levels is essential to mitigate climate change and promote sustainable agricultural development. The aim was to evaluate biomass production, soil C distribution and greenhouse gas emissions in a long-term (10 years) cover crop management system in the Cerrado.

Methodology: GHG emissions were analyzed during the soybean cycle on the biomass of cover crops in Rondonópolis – MT. The cover crops were: 1) Fallow; 2) Crotalaria spectabilis; 3) Urochloa ruziziensis; 4) U. brizantha (2 years) and maize/U. ruziziensis (7 years); 5) Cajanus cajan (2 years), Helianthus annuus/U. ruziziensis (3 years) and mix (C. spectabilis; P. glaucum; U.ruziziensis e C. cajan) (4 years). For each treatment, 4 replicates and 3 collection times (0, 15, and 30 min) were obtained using manual static chambers. The ppm gas concentration data obtained from the GC were converted to the mass of molecules of each gas per camera volume using the ideal gas law. The mass data were converted to gas flow per minute using linear projection and the concentrations of each gas for the three collections. To determine the total weight of biomass in the sampled area, the cover crops were cut close to the ground and the entire biomass of 1 m² was collected. After collecting the biomass, a sub-sample was taken, weighed and placed in a forced-air oven (55 °C) for 72 h and weighed again to obtain the dry matter, and then the total wet weight obtained in the field was adjusted to the amount of dry matter in kg ha-1.

Physical fractionation of SOM was performed, separating SOM into particulate organic matter (MOP) and mineral-associated organic matter (MOAM) (Cambardella and Elliott, 1992).

Preliminary results: The highest biomass (around 10 t ha-1) was produced by the U. ruziziensis, maize/U. ruziziensis and mix of cover crops. These are also the cover crops that had the highest soil C contents in the MOAM fraction.

POM is the fraction of organic matter that is the most sensitive to management practices and, as a result, can be easily lost. Compared to the soybean/fallow treatment, soybean/U. ruziziensis accumulated about 300% more C in the MOP fraction.

There was no difference in CO2 emissions between cover crops and fallow. The soil release an average of 2,500 kg C ha-1, with higher emission peaks during rainfall and lower soil temperature. This may have occurred because the fallow treatment did not control weeds, so it may have had biological activity to decompose the weed biomass. Similarly, greater quantity and quality of cover crop biomass resulted in higher MOP and MOAM than fallow.

The lowest emission of CH4 was produced by the biomass of U. ruziziensis and the highest emission of N2O was produced by the Mix, maize/U. ruziziensis and U. ruziziensis treatments

with an average emission of 450 g N ha-1. GHG release is a consequence of root respiration, microbial respiration, and soil carbon dynamics. Soil temperature and soil moisture are recognized as the main determinants of soil CO2 fluxes by controlling microbial activity and SOM decomposition.

Preliminary conclusions: However, soybean/U.ruziziensis showed the highest biomass production, higher C contents (g C/kg soil) in the MOP and MOAM fractions, and a soil sink for CH4. in addition to negative N2O fluxes through C. spectabilis. This assessment is essential for the calculation of the carbon balance of agricultural systems and for the definition of more promising management options for the mitigation of climate change. The data presented in this study are partial and refer to the year 2023/1, the study is ongoing and is expected to be completed in 2024/2.

Wanderlei Bieluczyk
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Abstract Title: On-field measurements of greenhouse gas fluxes in Brazilian low-carbon agriculture: a meta-analysis and critical insights

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Abstract: Regenerative low-C agricultural systems in Brazil offer a cost-effective and scalable nature-based solution to achieve net-zero GHG emissions. However, fragmented GHG research and incomplete on farm measurements of CO2, CH4, and N2O fluxes during system transitions lead to inaccurate net GHG estimates. This systematic literature review focused on GHG measurements in Brazilian low-C systems. Our objectives included refining GHG data, identifying organizations and authors, assessing distributions of studied GHG molecules, low-C system types, and productive components, conducting a meta-analysis on system conversion

effects, and providing methodological insights for future research. A thorough screening uncovered 78 relevant papers presenting fluxes measured on-farm out of 1,200 mentioning GHG and low-C systems. Most authors (91%) were Brazilian, with a notable influence from Embrapa and universities in the south, southeast, and central-western regions. Science mapping revealed a need for broader participation from northern and northeastern Brazil and international contributions. Most research focused on the Atlantic Forest and Cerrado, with limited data for Pantanal and Caatinga. Over half of the studies evaluated individual GHG molecules and single low-C systems. Urochloa spp. and Avena spp. were the most studied forage genera, while soybeans and corn dominated annual crops. Eucalyptus spp. and beef cattle were common trees and animals. No-till, integrated crop livestock, and integrations involving trees showed soil C-CH4 influx ranging from 0.8 to 1.0 kg ha-1 y-1. Converting managed pastures to integrated systems decreased N-N2O emissions by up to 1.63 kg ha-1 y-1, mitigating 700 kg CO2e ha-1 y-1. Overall, converting extensive grazed land to intensified or integrated systems lowered animal CH4 intensity, with cuts of up to 4.5 g CH4 per kg of dry matter intake and 122 g CH4 per kg of average daily weight gain. GHG flux units should be collaboratively standardized to turn magnitudes comparable since 8-10 units were used for each GHG molecule. We urge researchers to include crucial ancillary variables to help comprehend the soil GHG flux drivers. These variables were missing frequently; for example, soil bulk density and temperature were absent in over half of the studies. In conclusion, our literature review strongly indicates that adopting intensive and diversified low-C systems can significantly reduce GHG emissions, particularly the CH4 production per unit of beef meat. However, it's essential to exercise caution when extrapolating these findings, as the current data provides only a partial view of Brazilian edaphoclimatic conditions. This underscores the urgent need for conducting extensive on-farm GHG measurements across Brazil. Our findings suggest a need for better GHG protocol adherence or the development of an updated protocol for low-C tropical agriculture by specialists identified in our bibliometrics.

Keywords: Brazil, Regenerative Agriculture, GHG Flux Measurement, Integrated Farming Systems, Climate Change Mitigation.

Introduction and Objectives: Global warming and climate change have been driven by rising greenhouse gas (GHG) emissions in recent decades. To fight climate change, Brazil pledged at COP26, at the Glasgow Climate Pact, to halt illegal deforestation by 2028, cut GHG emissions by 50% by 2030 compared to 2005, and achieve net zero emissions by 2050. However, in 2021, land-use changes and agriculture accounted for 74% of Brazil's GHG emissions, with agriculture contributing 25% and releasing 600.8 Mt of CO2e, a 60.4 Mt increase compared to a decade ago.

Key sources of GHG emissions in Brazilian agriculture include cattle herds, fertilizer usage, animal waste management, irrigated rice cultivation, and residue incineration. Established low-C agriculture systems like no-till (NT) and well-managed pastures (MP) have helped mitigate GHG emissions to some extent. Given Brazil's status as the world's second-largest cattle ranching hub, transitioning animals to integrated farming systems like integrated crop-livestock

(ICL) and integrated crop-livestock-forestry (ICLF) could provide additional nature-based solutions to optimize land use and cut net GHG emissions. These systems align with agroecology principles, breaking away from conventional agriculture. Collectively, NT, MP, and integrated farming systems with (I.TREES) and without (ICL) trees have the potential to mitigate 164.3 million Mg CO2e between 2020 and 2030, according to the ABC+ Plan. However, further scientific validation through national data analysis is necessary, considering diverse soil and climate conditions and accounting for GHG emissions' warming potential. Given this, we conducted a systematic bibliometric review on GHGs (CO2, CH4, and N2O) and low-C systems in Brazil. It aimed to map scientific contributions, analyze study distribution, calculate GHG dynamics during transitions, identify methodologies, and highlight research gaps for future GHG studies in Brazilian low-C agriculture.

Methodology: A systematic review was conducted to gather GHG flux data (CO2, CH4, N2O) from Brazilian low-C agricultural systems. Scopus, Web of Science, and Dimensions databases were searched for English and Portuguese articles. The focus was on GHG flux assessments in Brazil, excluding gray literature and studies conducted outside Brazil or relying solely on models or lab work, resulting in 74 relevant articles. The 'bibliometrix' package in R software version 4.2.2 (2022) was used to merge, de-duplicate, and select relevant variables from an initial pool of 1924 documents. Following this process, 1200 documents remained, which underwent rigorous manual screening, resulting in the final selection of 74 documents for further analysis. Bibliometric and science mapping analyses were performed, tracking publication trends, author affiliations, keywords, and collaboration networks. Maps were created using QGIS 3.28 and R to visualize GHG assessments across Brazil and treatment distribution (MP, NT, ICL, I.TREES) across different biomes and altitudes.
In Excel, GHG molecule and system frequency were examined, and Venn diagrams were created for clarity. Production components within systems were documented, GHG flux units were standardized, and hourly and annual scale analyses were conducted, producing boxplot graphs in R. The analysis focused on five core system categories, calculating 95% confidence intervals, means, and upper/lower values for annual soil GHG fluxes.
For enteric CH4 studies, a dedicated metadata spreadsheet was created, categorizing emissions based on specific criteria related to beef cattle production, focusing on CH4 emission intensity. System conversion analysis paralleled the soil GHG analysis approach.
Study methodologies, including gas sampling methods, replicates, emission curve analysis, and parameters recorded during gas sampling and land-use changes, were critically assessed. The presence or absence of additional parameters required for each GHG molecule was noted, with radar graphs in Excel illustrating frequency occurrence.

Preliminary results:

Science Mapping:

Our study analysed articles on the influence of low-C agricultural systems on GHG emissions in Brazil. Publications on this topic grew annually by 12.9%, with 75% published from 2013 to

2022. Notably, 91% of the authors were from Brazil, with protagonist researchers affiliated with EMBRAPA, UFRGS, UFPR, and USP, among other institutions. The top five ranked collaborating authors were Bayer C, Piccolo MC, Carvalho AM, Zanatta JA, and Dieckow J, while Embrapa played a central role in institutional collaboration.

Distributions of studies:

NT and MP were more widely studied in Brazil, while ICL and I.TREES studies decreased. Most research focused on the Atlantic Forest and Cerrado, with the most limited data on Pantanal and Caatinga. 69% of studies examined GHGs separately, focusing on N2O (34%), CH4 (20%), or CO2 (15%) individually. 70% did not access more than one low-C agricultural system category (MP, NT, ICL, or I.TREES). The most studied forage genera were Urochloa spp. (26%) and Avena spp. (15%), and common annual crops included corn (43%) and soybeans (38%). Eucalyptus spp. was in 63% of studies, including trees, and beef cattle in 70% of grazed systems.

GHG Effects of System Conversion:

Soil CH4 influx was prevalent in NT and integrated systems. There was a shortage of year-long data to robustly cover the country's regional variations. Transitioning from negative controls

(degraded pastures or conventional tillage) to managed pastures increased C-CO2 and N-N2O emissions, mostly due to higher microbial activities and fertilizer usage. Nevertheless, converting MP to integrated systems decreased N-N2O emissions by up to 1.63 kg ha-1 y-1, mitigating 700 kg CO2e ha-1 y-1. Incorporating trees into ICL did not change annual soil GHG fluxes. For enteric CH4, converting degraded pastures to intensified or integrated pasture-based systems mitigated CH4 of up to 4.5 g per kg of dry matter intake and 122 g per kg of average daily weight gain.

Future methodology directions:

Most soil studies relied on chamber-based incubation measurements. Approximately 40% used only three points in time for emission curve regression, which may be insufficient according to GHG protocols. To improve this, we recommend a minimum of four samplings within a 40-60-minute timeframe for the vial approach. Among studies, eight to ten units were used to represent GHG fluxes for each molecule, complicating comparisons for readers. Collaborative efforts among low-C researchers are needed to standardize units. Essential ancillary GHG parameters like bulk density, temperature, and nitrogen, as well as desirable parameters like inorganic N forms alongside N2O fluxes, were missing in over half of the studies. Future research should incorporate these variables to better understand regulatory processes, enhance meta-analyses, and improve inventories and modelling.

Preliminary conclusions: Our findings about Brazil indicate an increase in GHG measurements in low-C systems in recent years, driven by the need for sustainable agriculture

to reduce emissions and sequester C, aiming for neutral or negative net GHG emissions. However, our comprehensive meta-analysis highlights a shortage in representing various systems and GHG molecules in year-long experiments. Therefore, we strongly encourage incorporating a broader range of low-C systems and GHG molecules in local experiments, leading to the identification of optimal sustainable farming practices. Including all three major GHGs (CO2, N2O, and CH4) allows for more reliable calculations of CO2 equivalence, net GHG flux, and C balance.

Considering the data limitations, our literature review strongly indicates that adopting intensive and diversified low-C systems can significantly reduce GHG emissions, especially CH4 production per unit of beef meat. However, we advise caution when extrapolating our meta-analysis results because the current data provides only a partial view of Brazilian edaphoclimatic conditions. This underscores the urgent need for extensive on-farm GHG measurements across Brazil. As our science mapping revealed, the country needs new researchers to contribute to the field, who can collaborate with the protagonist's authors and leading institutions we identified in the collaboration networks.

Our discoveries emphasize the need for better adherence to GHG protocols or developing updated protocols for low-C tropical agriculture, probably involving specialists identified in our bibliometrics. Collaborative efforts should address the complexity of GHG flux units and seek standardization consensus. Finally, we strongly encourage research colleagues to include essential ancillary data, at least in supplementary materials, to improve future meta-analyses, enhance understanding of key GHG flux drivers, increase inventory accuracy, and potentially aid predictive simulations (modelling).

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Abstract Title: Connecting carbon farming in Brazil and its implications for food (in)security in África

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Abstract: Carbon farming, also known as low-carbon agriculture, has gained significant attention in recent years as a potential nature-based solution to mitigate and adapt to the negative impacts of climate change on the environment. However, there is a common misconception that carbon farming practices oppose food security, which could hinder their widespread adoption. In this paper, we argue that carbon farming and food security are not opposing objectives but can be achieved simultaneously (in a synergic way) through the implementation of integrated agricultural systems (IAS). Integrated agricultural systems are promising land intensification/diversification strategies to produce food, feed, energy and sequester carbon in

the same area. Therefore, those systems can be both - a climate change mitigation and climate change adaptation strategy at the same time. Further, this paper will discuss carbon farming and practices including IAS in Brazil, which cover about 17 million ha, by reviewing scientific literature from scientific databases. The paper will also examine the implications of Brazilian carbon farming and IAS for food security in Africa by looking at the supporting policies, challenges, prospects, and way forward, as well as how these could be improved to support the nutritional needs of the rapidly growing African population.

Keywords: Food production; Low-carbon agriculture; Integrated agricultural systems; Nature-based solution; Brazil; Africa

Introduction and Objectives: In many African countries and in Brazil, agriculture and livestock are responsible for a substantial quantity of some GHGs (carbon dioxide (CO2), methane (CH4), and nitrous oxide (N2O)) which are emitted via carbon losses mainly induced by arable cropping, monocropping, deforestation, and changing land use to cultivation, as well as emissions originating from the use of synthetic fertilizers and by enteric fermentations of the livestock.

Further, poor farm practices such as the burning of agricultural waste, conventional soil tillage, and excessive irrigation also contribute to the emissions of the GHGs. For example, according to IPCC (2022), an estimated large amount of 22% of global GHGs emissions generally emanate from Agriculture, Forestry, and Other Land Use (AFOLU) with agriculture, deforestation, and intensive land use change as the main culprits. In Brazil, Land Use Change and Forest, and Agriculture sectors accounts for about 75% of national GHG emissions (SEEG, 2023).

But this could be radically different, as agriculture and livestock could reduce their GHG emissions and also, at the same time, serve as a significant carbon sink mechanism. If well and widely implemented, agricultural practices have the potential to sequester hundreds of billions of tons of carbon from the atmosphere in the coming years and decades.

Many studies have revealed that farmers can improve the quantity of carbon stocked in agricultural soils and decrease the rate of carbon emitted back into the atmosphere through these carbon farming approaches

These include the IAS that combine at least two farming practices: a) crops and animals on the same piece of land (ICL); b) crop and forest (ICF); c) livestock and forest (ILF); d) or the more integrated form crop with livestock and forestry (ICLF). IAS as a key system for carbon farming can also include crop rotation, intercropping, improved fallow, and agroforestry systems (alley cropping, silvopasture, silvoarable, silvohorticulture), forest farming, shaded-perennial cropping, as well as some other adopted joint crops and livestock practices namely, homegarden, apiculture, hedgerows.

Methodology: This work aims to contribute to closing the knowledge gap by clarifying that carbon farming and food security are not opposing objectives but can be achieved simultaneously through the implementation of IAS. This work's main aim and associated

specific objectives of this work are met by dividing the paper into seven sections.
The first and second sections involved the introduction and conceptual/theoretical framework. The relationships between IAS and carbon farming, as well as carbon farming practices that enhance food production, are discussed in sections 3 and 4. In the fifth section, food (in)security in Africa was demonstrated using a comparative analysis with the outside world.
The main drivers and victims of food insecurity in Africa were examined in section 6. The seventh section of this work provided highlights on the implications of Brazilian carbon farming and IAS for food security in Africa by focusing on the supporting policies, challenges, prospects, and way forward as well as how these could be improved to support the nutritional needs of the rapidly growing African population. The transfer or cycling of CO2/carbon between the atmosphere, plants and soil ecosystems involves dynamic and complex processes which are strongly interlinked and are significantly controlled by diverse drivers
Carbon enters the soil from the atmosphere through photosynthetic plants as root exudates or via root or aboveground biomass decomposition. In the soil, carbon occurs in root or microbial biomass, as bioavailable labile organic carbon, or as more recalcitrant carbon. In the biotic components, carbon is shared among the various living plant pools, primarily leaves, stems and roots which are the donor pools.
Subsequently, from the plants (the donor-pools), and via decomposition, exudation, and sequestration, carbon is released to the recipient-pools (namely litter and soil pools), which largely depends on the amount absorbed and released from the plant stocks. Carbon leaves the soil as direct emissions, or via root or microbial respiration, and microbial-mediated soil respiration is the major source of carbon emission (CO2) from terrestrial ecosystems.

Preliminary results: The Brazilian National Policy on Climate Change (BPNMC) creates some voluntary targets to mitigate climate change by increasing carbon stocks and reducing GHG emissions as pledged at the United Nations Framework Convention on Climate Change (UNFCCC). The BPNMC regulations stipulated the allotment of targets and indicators for the prediction and estimation of targets and for the development of sectoral strategies for emissions reduction between 36.1% and 38.9% of the total annual emissions. The strategy for the mitigation aimed at the 2020 targets was allocated among four socioeconomic sectors of the nation including, (i) change in the use of land and forests, (ii) agriculture, (iii) energy (iv) industrial processes and waste treatment (Table 3).In this voluntary mitigation target the agricultural sector and changes in land and forest use were among the top target areas for achieving the goals with agriculture's projections at 730 million tons of CO2eq while change in land and forest use was 1,404 million tons of CO2eq. These target values brought significantly positive changes in policies for agriculture, forests, and land use. Top among the policies and programs was the Low-Carbon Agriculture Plan, which is commonly referred to as the ABC Plan, created in 2010. The agricultural ABC plans as the sector-based strategies from the BPNMC to mitigate climate change by increasing carbon stocks, and reducing or preventing GHGs emissions involved some set of action goals which among others include: (1) restoration of degraded pastures, (2) development and enhancement of organic agricultural systems (3) formation and promotion of no-till cultivation and sowing systems, (4) creation and

enhancement of IAS referred as the ABC Integration which among others consisted of integrated crop-livestock-forest, livestock-forest, crop-livestock, crop-forest integration, and integrated agroforestry systems. These policies and practices have to a large extent supported Brazil in reaching their present position as one of the top countries with high agricultural production, and with enough food to support the low food producing countries in Africa as part of the Brazilian foreign policy approach to increment Global South cooperation based on solidarity and mutual interests, which includes the potential of transfer of technology in carbon farming. Carbon farming in Brazil and globally has large environmental and socioeconomic benefits, and challenges as have been highlighted in this section.

Preliminary conclusions: Carbon farming is a potential nature-based solution to mitigate climate change by reducing excess atmospheric CO2 and storing it in the soil and plants while minimizing GHG emissions. However, some people have erroneously believed that carbon farming practices are against food security, and this misconception should be discarded based on the benefits of carbon farming, as discussed in this work. This work acknowledged that the transformation of agriculture towards a carbon farming system is strongly linked with IAS with the primary aim of enhancing food security by transforming production and consumption processes.
This paradigm shift in farming simultaneously reduces GHGs emissions, improves soil health, minimizes waste and ineffective use of natural resources, increases biodiversity, and enhances energy security. The necessity for carbon farming in Brazil results from the internal efforts of the Brazilian government through the IPCC-NDC agreement, which metamorphosed into the establishment of climate change mitigation via the agricultural sector, thus, the adoption of the ABC plans and policies. Since its creation, the ABC schemes have significantly promoted Brazil to the position among the top countries in the world with reasonable food for its populace as well as to support other nations in Africa. On the one hand, the complementarity of carbon farming and IAS and the adoption of sustainable farming practices in Brazil to tackle the food insecurity problem in Africa caused by human and natural factors; on the other hand, it will contribute to a strong synergy for addressing food (in)security in Africa. However, improved food production through IAS powered by carbon farming in Brazil could support high nutritional demands in Africa yet, most of the drivers of food insecurity in the region need to be addressed to enable the people to be self-dependent and cope with the present and future scenarios.

Dener Oliveira
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Abstract Title: Make the data available: an analysis of the soil C research for the Brazilian Cerrado

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Abstract: There is a plenty of available data regarding the effects of land use and management practices on the soil C stocks across Brazilian Cerrado. However, the lack of methodological standardization and the unavailability of raw data and basic explanatory variables [i.e., time span, soil C content (SOC), bulk density (Bd), temperature, precipitation, and soil texture] precludes broader applications for such a valuable dataset. Here, by a systematic review of 87 papers, we evaluate how available are the data of soil C research in Brazilian Cerrado. Most of the studies assembled here reported soil C stocks, but did not provide raw data or important ancillary/explanatory variables. About half of the studies did not provide the primary data on SOC and Bd, both used to calculate soil C stocks. Moreover, for more than 40% of the papers, there is no information regarding the time since the adoption of the evaluated practice. Actually, a few studies provided detailed information about land-use history and management. On the other hand, most of the studies presented mean temperature and precipitation for the sites evaluated. Surprisingly, clay content values were reported for every plot and soil depth in only 18% of the studies. Recognizing the importance of using the available soil C stocks for greenhouse gases inventories and also on climate policy, we ask colleagues to include the primary dataset (e.g., SOC) and the explanatory variables (e.g., clay content) at least in the supplementary material. Likewise, it is important that studies report the time span since the adoption of a practice whenever possible. Obtaining information on soil C stocks is often arduous, costly and time-consuming. We must make it available! Increased cooperation, higher trust in the results, and goodwill among scientists are just a few of the benefits. Specifically, methodological standardization and provision of detailed information would represent a major improvement in C inventories, meta-analysis or simulation (modelling) efforts to draw general conclusions and support climate policy in Brazilian Cerrado.

Keywords: climate change, open science, raw data, C inventories, land use.

Introduction and Objectives: There is a plenty of available data regarding the effects of land use and management practices on the soil C stocks across Brazilian Cerrado. However, the lack of methodological standardization and the unavailability of raw data and basic explanatory variables [i.e., time span, soil C content (SOC), bulk density (Bd), temperature, precipitation, and soil texture] precludes broader applications for such a valuable dataset.

Methodology: Here, by a systematic review of 87 papers, we evaluate how available are the data of soil C research in Brazilian Cerrado.

Preliminary results: Most of the studies assembled here reported soil C stocks, but did not provide raw data or important ancillary/explanatory variables. About half of the studies did not provide the primary data on SOC and Bd, both used to calculate soil C stocks. Moreover, for

more than 40% of the papers, there is no information regarding the time since the adoption of the evaluated practice. Actually, a few studies provided detailed information about land-use history and management. On the other hand, most of the studies presented mean temperature and precipitation for the sites evaluated. Surprisingly, clay content values were reported for every plot and soil depth in only 18% of the studies. Recognizing the importance of using the available soil C stocks for greenhouse gases inventories and also on climate policy, we ask colleagues to include the primary dataset (e.g., SOC) and the explanatory variables (e.g., clay content) at least in the supplementary material. Likewise, it is important that studies report the time span since the adoption of a practice whenever possible.

Preliminary conclusions: Obtaining information on soil C stocks is often arduous, costly and time-consuming. We must make it available! Increased cooperation, higher trust in the results, and goodwill among scientists are just a few of the benefits. Specifically, methodological standardization and provision of detailed information would represent a major improvement in C inventories, meta-analysis or simulation (modelling) efforts to draw general conclusions and support climate policy in Brazilian Cerrado.

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Abstract Title: Land use intensification as a strategy to increase soil carbon storage and stabilization in tropical conditions

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Abstract: Intensifying land use systems using brachiaria grass (Brachiaria brizantha) can be a promising nature based solution to increase carbon (C) sequestration in tropical soils. The main objective was to quantify soil C changes, and understand the mechanisms of soil C storage and stabilization under distinct land use configurations. A field experiment was conducted for 11 years in a randomized block design with four replications at Sinop/MT−Brazil. Four treatments were evaluated: Crop Succession (CS) – annual cultivation of soybean followed by corn +

brachiaria in the inter-row; Integrated Crop-Livestock (ICL) – a four-year rotation system with soybean/corn + brachiaria in the first and second years, followed by more two years of brachiaria under cattle grazing; Integrated Crop-Livestock-Forest (ICLF) – a ICL system with an additional forest component with eucalyptus; and a well-managed Pasture (MP) – continuous cultivation of brachiaria with cattle grazing. Soil samples were collected up to a 100 cm depth at each system. At ICLF, soil samples were collected below the eucalyptus row, and in the inter-row position (between ranks), and the results were treated as a weighted average of the positions (30% of the area in row and 70% in inter-row). The total C concentration was quantified by dry combustion, aggregate stability was analysed by wet-sieving, and the chemical surface composition of C was determined by x ray photoelectron spectroscopy. The different land-use configurations significantly affected C stocks at surface layer. The treatments ICL and MP showed higher soil C stocks compared to ICLF and CS in the 0-5 and 5-10 cm depths. Considering the layer of 0-10 cm, soil C stocks of 30.9, 29.7, 36.5 and 39.4 Mg ha-1 were observed in CS, ICLF, ICL and MP, respectively. In the ICLF system, the soil C stocks in eucalyptus row were 26% lower than the inter-row at 0-5 cm layer. Higher aggregate stability was observed under MP and ICL at 0-5 cm layer, and they were positively correlated with soil C stocks. The high-resolution C spectra data showed notable increase in the relative abundance of recalcitrant C groups (aliphatic/aromatic) in soils under MP and ICL by 17 and 9% compared to ICLF and CS at 0-5 cm layer, respectively. Our findings indicate that the land use systems with greater use of brachiaria (in time and space) resulted in high C stocks and high chemical recalcitrance. We concluded that brachiaria grass, either in well-managed pastures or integrated systems, can be considered good options to increase and stabilize C in tropical soils. The results presented herein provide a scientific basis for a comprehensive understanding of soil C sequestration mechanisms in Brazilian agriculture.

Keywords: soil aggregation; XPS; brachiaria; carbon sequestration.

Introduction and Objectives: Intensifying land use systems using brachiaria grass (Brachiaria brizantha) can be a promising nature based solution to increase carbon (C) sequestration in tropical soils. The main objective was to quantify soil C changes, and understand the mechanisms of soil C storage and stabilization under distinct land use configurations.

Methodology: A field experiment was conducted for 11 years in a randomized block design with four replications at Sinop/MT−Brazil. Four treatments were evaluated: Crop Succession (CS) – annual cultivation of soybean followed by corn + brachiaria in the inter-row; Integrated Crop-Livestock (ICL) – a four-year rotation system with soybean/corn + brachiaria in the first and second years, followed by more two years of brachiaria under cattle grazing; Integrated Crop-Livestock-Forest (ICLF) – a ICL system with an additional forest component with eucalyptus; and a well-managed Pasture (MP) – continuous cultivation of brachiaria with cattle grazing. Soil samples were collected up to a 100 cm depth at each system. At ICLF, soil samples were collected below the eucalyptus row, and in the inter-row position (between ranks), and the results were treated as a weighted average of the positions (30% of the area in row and 70% in

inter-row). The total C concentration was quantified by dry combustion, aggregate stability was analyzed by wet-sieving, and the chemical surface composition of C was determined by x-ray photoelectron spectroscopy.

Preliminary results: The different land-use configurations significantly affected C stocks at surface layer. The treatments ICL and MP showed higher soil C stocks compared to ICLF and CS in the 0-5 and 5-10 cm depths. Considering the layer of 0-10 cm, soil C stocks of 30.9, 29.7, 36.5 and 39.4 Mg ha-1 were observed in CS, ICLF, ICL and MP, respectively. In the ICLF system, the soil C stocks in eucalyptus row were 26% lower than the inter-row at 0-5 cm layer. Higher aggregate stability was observed under MP and ICL at 0-5 cm layer, and they were positively correlated with soil C stocks. The high-resolution C spectra data showed notable increase in the relative abundance of recalcitrant C groups (aliphatic/aromatic) in soils under MP and ICL by 17 and 9% compared to ICLF and CS at 0-5 cm layer, respectively.

Preliminary conclusions: Our findings indicate that the land use systems with greater use of brachiaria (in time and space) resulted in high C stocks and high chemical recalcitrance. We concluded that brachiaria grass, either in well-managed pastures or integrated systems, can be considered good options to increase and stabilize C in tropical soils. The results presented herein provide a scientific basis for a comprehensive understanding of soil C sequestration mechanisms in Brazilian agriculture.

0811 - PS22 (TV2)

Chairs: Maurício Salles – Renato Monaro

Antônio Carlos Bastos de Godoi
USP

Abstract Title: Cyber Defense System for Smart Grid Communications

Authors' Names & Affiliation Institutions of all authors (in order for publication): Universidade de São Paulo.

Abstract: Power grids are evolving toward intelligent networks that integrate numerous renewable sources, sustainable power generation, and operational infrastructure to provide new capabilities, reduce emissions, enhance efficiency, and improve energy conservation. To accomplish the business goals of smart energy systems, a sophisticated ecosystem of computation, networking, robotics, cloud computing, and the Internet of Things are incorporated, reducing the isolation, increasing the attack surface, and making the industry

highly vulnerable to cyberattacks. In this scenario, cybersecurity
emerges as a prominent issue, demanding innovative solutions to defend against the attacks increasing in frequency and sophistication. In this work, we illustrate the use of a cyber defense model based on stochastic cellular automata to contain the spreading of malware in a smart grid. Numerical simulations consistently showed the effectiveness of the strategy to mitigate the attack, reducing the number of infected. Additionally, cellular automata could implement the model's algorithm while adequately representing this kind of infrastructure, where the topological characteristics and locality principle are very prominent.

Keywords: Cyber Security - Malware - Smart Grids.

Introduction and Objectives: The sustainable modernization of the energy sector moved the industry to the next stage of evolution, whereby it has undergone technological changes to become increasingly similar to corporate IT. As the interconnectedness marches on, the risks and possible impacts increase as they are not only limited to the service provider but also extended to the economy.
In this work, we illustrate the use of a mitigation strategy based on stochastic cellular automata to effectively contain the spreading of malware in a smart grid infrastructure.

Methodology: The performance of the model is evaluated by running a computer simulation of a hypothetical cyberattack and defense scheme in a smart grid infrastructure.

Preliminary results: The computer simulations demonstrated that increasing the probability of the susceptible nodes detecting infected neighbours flattens the curve of infection over time.

The study showed that by properly choosing the set of parameters, the containment model reaches an optimal response, capable of reverting the initial high infection rate toward a sustained decreasing trend.

Preliminary conclusions: This work presents an early warning framework for forecasting malware attacks. The model is capable of mitigating the cyberattack as alerted systems can employ defense measures to reduce their risk of infection. This scheme can be appropriately used in smart grid infrastructures, which require a timely response to security events, enabling them to react beforehand, preventing malicious attacks from spreading, enhancing security, and protecting the privacy of the users.
Numerical simulations revealed that the strategy is able to contain the spreading, resulting in a smaller number of infected and fewer regions affected. In a modern scenario where the industry is enduring demanding security challenges to keep in pace in terms of preparedness, this model presents a plausible alternative to help reduce the contemporary threats facing the energy sector.

Beatriz Aline Riga Rocha
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Abstract Title: Investigation of Ni and Cu doping effects on the sintering and proton conducting behaviour of BaZr0.7Ce0.2Y0.1O3-δ

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Abstract: BCZY (BaZr0.7Ce0.2Y0.1O3-δ), a commercial protonic electrolyte, was modified by doping with CuO or NiO (1 wt.%), aiming to improve the sintering behaviour of the electrolyte. As expected, the transition metals acted as sintering aids. Due to their presence, the sintering occurred at 1350 °C (with Cu) and 1450 °C (with Ni) at six h. A greater degree of densification was observed for the modified materials but not for the pristine BCZY at the same conditions. The electrical results reveal that the protonic conduction characteristic was maintained for the Ni-dopped material. Meanwhile, the electronic and anionic conduction seems predominant for the Cu-doped one.

Keywords: BZCY, protonic electrolyte, transition metal doping, SOFC, SOEC.

Introduction and Objectives: As an excellent alternative for electric energy generation, the use of ethanol in fuel cells, which can either work as a solid oxide fuel cell (SOFC) or as a solid oxide electrolysis cell (SOEC), has been seen as a significant advance. Despite the advantages of clean energy and environmental friendliness provided by these systems, the need to operate at high temperatures (800-1000 °C) instigates efforts to optimise and improve their energy conversion efficiency.

Nowadays, most conventional solid oxide electrolytes are oxygen-ion conductors, which can only reach sufficient ionic conductivity at high temperatures. Accordingly, the interest in proton-conducting electrolytes has increased due to their relatively lower activation energy and higher conductivity at intermediate low temperatures (400-700 °C).

Currently, the main protonic electrolytes known are the metal oxides with perovskite structure of the type A2+B4+O3, in which the A2+ sites are occupied by divalent cations (such as Ca2+, Ba2+ and Sr2+), and the B4+ sites are occupied by tetravalent cations (such as Zr4+ and Ce4+; respectively known as zirconates and cerates). Among these two classes, ceramics based on cerates have the highest proton conductivity at intermediate temperatures (400-800°C) despite presenting low chemical stability. On the other hand, zirconates, although having good chemical and thermal stability, show conductivity values not as high as the ones offered by the prior compounds at the same conditions. Merging the advantages of cerates and zirconates, solid solutions of BaCeO3 BaZrO3 have been developed to balance conductivity and chemical

stability. Examples of these types of materials are compounds with the general formula BaZrxCeyYzO3-δ, e.g., BaZr0.7Ce0.2Y0.1O3-δ. Notwithstanding the improvements achieved by the combination of Ce and Zr, some issues are still to be addressed, such as high grain boundary resistance and elevated sintering temperatures for densification. In this scenario, this work aims to investigate the optimization of the sintering behavior and electrochemical characteristics of the commercial electrolyte BaZr0.7Ce0.2Y0.1O3-δ (BZCY) through its modification by the addition of sintering aids.

Methodology: To prepare the modified materials, pristine BZCY (BZCY721, FuelCell Materials) and 1 wt.% of NiO (99.8%, Aldrich) or CuO (97.8%, Aldrich), were wet ground in a zirconia mortar using isopropanol as the medium. The obtained powders were pressed into pellets under 196 MPa using a 19 mm diameter stainless steel die. The pellets were sintered in air at 1450 °C (for NiO) and 1350 °C (for CuO) for 6 h. Standard pellet samples were prepared in the same conditions, but in the absence of sintering aids (NiO or CuO), with 100% of pristine BZCY, and were sintered at 1350 and 1450 °C for comparison purposes. It is worth mentioning that, for the sintering process, each pellet was embedded with powders of the same type to prevent elemental volatilization. Samples of BZCY721 (as received) and BZCY721 containing 1 wt.% of NiO or 1 wt.% of CuO are noted as BZCY, BZCY Ni and BZCY Cu, respectively. The physical characteristics of the samples were investigated by scanning electron microscopy (SEM). The electrical properties of the BZCY-Cu and BZCY-Ni were assessed by electrochemical impedance spectroscopy. The AC impedance spectra were obtained at a 400 800 ºC and under dry-H2 and wet-H2 atmospheres.

Preliminary results: After the sintering process at each respective temperature, the BZCY (1350 and 1450 °C), BZCY Cu (1350 °C) and BZCY Ni (1450 °C) materials presented average sintering values of 10.2%, 15.2%, 25.5% and 26.8%, in this order. These values indicate that the electrolyte exhibits higher thermal contraction behaviour in the presence of the transition metals Cu and Ni. Agreeing to that, the cross-sectional SEM images revealed that the BZCY, without any sintering aid, developed smaller grains and presented larger pores compared to the BZCY Cu and BZCY Ni. Additionally, the SEM data confirm that the temperature also plays an important role in the densification of the BZCY. For the BZCY sintered at 1450 ºC, grain growth and decrease in porosity were favoured compared to the BZCY sintered at 1350 ºC. Besides the slightly larger shrinkage value presented by BZCY-Ni, compared with BZCY-Cu, its microscopy images indicate more significant densification for this material.

The conductivities (σ) for the BZCY Cu and BZCY Ni materials were calculated from the AC impedance spectrum. For both of them, the total conductivity values under wet-H2 atmosphere were higher than those under dry-H2. At 600 ºC, BZCY-Cu exhibited σ = 3.87 mS cm-1 (wet-H2) and σ = 3.36 mS cm-1 (dry H2), whereas BZCY-Ni showed σ = 2.45 mS cm-1 (wet-H2) and σ = 0.24 mS cm-1 (dry-H2). As represented by these values, the difference between the conductivity under wet and dry H2 atmospheres was greater.

Analyzing the activation energy (Ea), determined from the Arrhenius plot of the total conductivity data for BZCY-Ni, a decrease in Ea is observed under H2 atmosphere containing

water: Ea,wet = 0.12 eV < Ea,dry = 0.31 eV. This result, associated with increased conductivity under the same atmosphere, confirms that BZCY-Ni is mainly a proton conductor material in these conditions. On the other hand, for the BZCY-Cu under wet-H2, the Ea value is slightly larger than the one in dry atmosphere (Ea,wet = 0.13 eV > Ea,dry = 0.16 eV), indicating that, for this material, electron-hole and oxygen vacancies are likely to be the main charge carriers in this environment.

Preliminary conclusions: According to the preliminary results, the addition of CuO and NiO, even in concentrations as small as 1 wt.%, is capable of favouring the sintering process, allowing the BZCY721 to achieve a higher degree of densification at relatively lower temperatures. In the case of the BZCY-Ni material, the electrical investigation returned an increase in conductivity followed by a decrease in the activation energy. Such observation confirms that, despite the Ni addition, the electrolyte BZCY-Ni maintained its proton conductivity behavior under humidified H2 atmosphere. Conversely, BZCY-Cu, under wet-H2, presented only a moderately larger conductivity associated with a slight increase in the activation energy, which might be related to electronic and anionic conduction.

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Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Wind potential improvement through the study and mitigation of generation deviations and failures.

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Abstract: This research project aims to improve the use of the wind resource by achieving the following objectives: (i) production of artificial intelligence (AI) tools to characterize deviations between forecast and generation, identifying their probable causes, (ii) production

of AI tools for the diagnosis and prognosis of mechanical and electrical failures and development of an advanced framework of predictive maintenance, (iii) production of AI tools that allow identifying and classifying damage on the surfaces of wind turbine blades based on the processing of images captured in the field, and (iv) updating the energy conversion models with the tools and knowledge resulting from the previous objectives. The final products of this project will be a set of methodologies and software, tested, validated and ready to be used. They will have the potential to generate significant impact for the business because, by mapping wind turbine failures and their causes, they will enable the implementation of more efficient operation and maintenance procedures, which will lead to an increase in the capacity factor, energy efficiency and lifespan of wind farm assets.

Keywords: Wind power, Operation and maintenance, Data science, Predictive maintenance.

Introduction and Objectives: This research project aims to improve the use of the wind resource by achieving the following objectives: (i) production of artificial intelligence (AI) tools to characterize deviations between forecast and generation, identifying their probable causes, (ii) production of AI tools for the diagnosis and prognosis of mechanical and electrical failures and development of an advanced framework of predictive maintenance, (iii) production of AI tools that allow identifying and classifying damage on the surfaces of wind turbine blades based on the processing of images captured in the field, and (iv) updating the energy conversion models with the tools and knowledge resulting from the previous objectives. The final products of this project will be a set of methodologies and software, tested, validated and ready to be used. They will have the potential to generate significant impact for the business because, by mapping wind turbine failures and their causes, they will enable the implementation of more efficient operation and maintenance procedures, which will lead to an increase in the capacity factor, energy efficiency and lifespan of wind farm assets.

Methodology: The solution will be composed of sensors and field instrumentation, local high performance processing server, remote cloud server, massive data analysis software and web software for remote access to information for intelligent auditing of the assets. Among the specific objectives is the evaluation of the regulatory framework and the prediction of revenue loss for failure and maintenance intervals and frequencies, as well as the impact of increased availability on the plant's revenue. Thus, this project will provide the diagnosis and present ways to increase the revenue of the wind power generation business in an integrated manner, streamlining decision making. The proposed work is at the frontier of knowledge of the application of computational modelling and simulation, big data and artificial intelligence to the wind energy sector, by using techniques that are currently being established in the academic and technical community and using a global monitoring dataset that is being built in the industry and enables a myriad of applications that are beginning to be explored.

Preliminary results: The project has just started.

Preliminary conclusions: The application in the operation and maintenance division is immediate, with gains to be realised in the short to medium term. These are relevant developments for energy companies, which increase the profitability of the business, but also bring benefits to society in general, by increasing energy security and decreasing the cost of a clean energy source. From their conception, the products of this project will be designed for large scale, taking as a premise that hundreds of wind turbines will be monitored simultaneously. This facilitates a very favourable financial return, since the cost of replacing a large component of a single wind turbine is in the order of millions of Brazilian Reais. The costs of this project will be compensated if three or four breakdowns are avoided over the next few years, not to mention the productivity gains and savings in the operation of the park. This shows that the project has excellent cost reasonability.

Carlos Andre Persiani Filho
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Abstract Title: UAV-Assisted Fault Detection in Electrical Distribution Systems

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Abstract: In onshore wind farms, electrical distribution systems are susceptible to several damaging effects, potentially leading to faults that pose critical safety concerns. Once the fault location is identified, prompt detection becomes paramount to ensure the safe resumption of system operations. To address this issue, a UAV-based system is to be conceptualized for the automatic detection and reporting of faults. A DJI Matrice quadcopter is equipped with both RGB and thermal cameras, forming the sensor platform for environmental sensing. A path planning model is employed to determine the positions and orientations of both the drone and sensors, enabling effective monitoring. Additionally, a deep learning algorithm is utilized to

detect fault types. The neural network can operate in real-time or offline. Further, a computational scenario is designed to simulate the system operation. We aim to test the effectiveness of our automatic detection model in real-life tests.

Keywords: UAV Path Planning; Deep Learning; Defect Detection; Transmission Line Fault Detection.

Introduction and Objectives: Our objective is to establish an end-to-end framework for UAV-assisted fault detection in electrical distribution systems. The UAV flight path model should consider the potential hazards posed by transmission lines. Also, the flight mission needs to incorporate a schedule for embedded sensors to monitor the environment. We will utilize deep learning techniques to extract fault types from the collected data. Additionally, a computational simulation will be designed to validate the framework concept safely. Ultimately, our goal is to test the proposed model in real-life scenarios.

Methodology: First, we conduct a bibliographical review with a focus on four primary aspects of the project: (1) Fault detection methods; (2) UAV Path Planning methodologies; (3) Computational Simulations; and (4) Embedded systems. This review highlights the most commonly employed strategies for each task. Further, we develop a trajectory algorithm to balance a safe flight path. The distance from the transmission lines plays a crucial role, as flying farther reduces electromagnetic interferences but limits sensor reach. We then create a virtual environment to simulate the testing system and prove the mission. Finally, we plan to allocate an embedded platform on a DJI Matrice 350 drone to conduct real life experiments for validating the proposed model.

Preliminary results: As this work is currently underway, we have not yet obtained any results.

Preliminary conclusions: As this work is currently underway, we have not reached any

conclusions yet.

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Abstract Title: Parameter estimation of power transmission systems by using least square methods and optimum filtering theory

Authors' Names & Affiliation Institutions of all authors (in order for publication): Polytechnic School - University of São Paulo POLI-USP

Abstract: A summarized review is presented on the Least Square Methods and Optimum Filtering Techniques applied for estimation of electrical parameters of power transmission systems. The estimation of such parameters, from accessible and periodic measurements, represents an efficacious procedure for continuous monitoring and reliability assessment of power systems in general.

Keywords: power systems; power transmission; parameter estimation; optimization.

Introduction and Objectives: The estimation of the electrical parameters of overhead transmission lines and cables represents an initial step for evaluation of entire power grids. These parameters are variable with the time, i.e. the impedance and admittance parameters are sensitive to the aging, degradation and defects on conductors and cables which compose the electric power systems. In this sense, a review on existing techniques for parameter estimation is carried out on, more specifically on the Least Square Methods and advanced techniques by using optimum filtering.

Methodology: A bibliographic review is presented based on the well-established literature and the state of the art.

Preliminary results: Technical articles and published results are presented and discussed, in order to validate the proposal on real time monitoring based on parameters estimation of power transmission systems.

Preliminary conclusions: The electric parameters of power transmission systems can be estimated, based on noisy current and voltage signals, by using different methods. The Least-Square method and Kalman Filter seems to be a robust solution, especially when combined with other heuristic and machine learning techniques.

Emanuel Percinio Gonçalves de Oliveira
São Carlos Engineering School

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Methodology for Obtaining an Intelligent Tool for Classifying Faults in Overhead and Underground Distribution Lines with High Penetration of Wind Sources Interfaced by Inverters

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Abstract: This work explores the growing demand for integrating renewable energy sources into power generation and distribution systems. Specifically, it focuses on the challenges associated with Wind Power Sources Interfaced by Inverters (WPSIIs) and their impact on fault classification within these systems. The type of faults in power systems is crucial for maintaining grid stability and reliability. Still, the introduction of WPSIIs has introduced new complexities due to the dependence on inverter control methods. In recent years, this topic has garnered increased attention in academic circles. However, the literature addressing the impacts of WPSIIs on fault classification still needs to be improved, and viable solutions still need to be improved. In this context, this research proposes using intelligent algorithms, specifically machine learning algorithms, as potential solutions to enhance fault classification in WPSII-integrated systems. The study will evaluate machine learning algorithms trained using signals generated through computer simulations with the PSCAD software. By comparing the performance of these algorithms, we aim to identify the method with the highest potential for effectively classifying faults in systems featuring WPSIIs. In conclusion, this work will provide valuable insights into the challenges posed by integrating wind energy sources into power systems and the potential of machine learning algorithms to enhance fault classification. It underscores the importance of addressing these challenges to ensure the continued reliability and stability of power grids in the context of renewable energy integration.

Keywords: Wind sources interfaced by inverters, Machine learning, Discrete wavelet transform, Fault diagnosis.

Introduction and Objectives: The way society obtains, stores, and consumes energy is of such importance that it is used as a significant factor in representing the technological development of a community. With scientific and industrial progress, new methods of generating and storing energy have been developed, bringing new challenges to distribution systems and demanding better strategies to ensure these systems' sustainable protection and operation. Furthermore, with the perils associated with the climate crisis, adopting renewable energy sources has increased worldwide. In particular, there is a strong presence of Wind Power Sources Interfaced by Inverters (WPSIIs) in the conventional transmission grids of various countries, especially Type III WPSIIs, or Doubly Fed Induction Generators (DFIG), and Type IV WPSIIs, or Full-Converter Generators (FCG). In Brazil, reports from the Energy Research Company indicate an increase in wind energy generation of over 20,000 GWh in just the last two years,

challenging conventional strategies for dealing with transient disturbances in the distribution system. In this context, the Brazilian National Electric System Operator (ONS) introduced Fault Ride-Through requirements for wind generation systems, representing the ability of electrical devices to remain connected to the grid and operate during periods of low voltage at the point of connection caused by faults. This change in network procedures has triggered a scientific and industrial demand for improved methods for fault assessment in WPSIIs. Considering the challenges posed by the increasing integration of WPSIIs in fault classification within distribution systems and the potential of intelligent solutions in addressing this issue, the primary objective of this project is to implement a machine learning-based model for fault classification in overhead and underground distribution lines with high WPSII penetration. This approach extends beyond the models already presented in the literature, such as Random Forest, Gradient Boosting, and Stochastic Gradient Descent Classifier.

Methodology: The project's first stage involves theoretical and practical aspects, focusing on analysing the distribution system through computer simulations performed using the Power Systems Computer Aided Design (PSCAD/EMTDC) software. This software specializes in simulating electromagnetic transients. The simulation will be designed to represent a test system encompassing the collector network of an onshore wind farm, with a specific emphasis on the medium-voltage overhead and underground distribution system. Various signal preprocessing tools will be explored within the simulated voltage and current oscillograph signals. These tools include the Wavelet Transform (WT), Continuous Wavelet Transform (CWT), and Stockwell Transform (ST), among others. The objective is to extract pertinent information from the system in the time, frequency, and time-frequency domains. Subsequently, the project aims to implement machine learning algorithms for fault classification. Different machine learning models available in the Python programming language's Scikit-learn library will be evaluated in this context. Scikit-learn provides various tools to enhance algorithm performance in data processing and model fine-tuning. Faults will be classified based on their nature, whether single-phase (involving one phase and ground, such as AT, BT, and CT), two-phase (involving two phases or two phases and ground, such as AB, AC, BC, ABT, ACT, BCT), or three-phase (involving all three phases, ABC). Once the analyzed algorithms are trained and tested, each will be evaluated based on three criteria: accuracy, precision, and training time. This evaluation will be facilitated by statistical tools such as confusion matrices and graphical representations. Ultimately, the aim is to determine which algorithms demonstrate the most significant potential for fault classification in Wind Power Sources Interfaced by Inverters (WPSIIs) with overhead and underground distribution lines.

Preliminary results: As the project has just started, it has not been possible to implement and obtain preliminary results concerning the proposal presented initially. The research is in the initial phase of bibliographical review, and the resulting results will be reported later.

Preliminary conclusions: As mentioned earlier, the project has just started, and it has not been possible to obtain preliminary conclusions. The resulting analysis will be reported later.

Enrique Adalberto Paredes Salazar
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Abstract Title: Understanding Electrocatalytic Reactions trough Microkinetic Modelling Approaches

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Abstract: A profound comprehension of the intricate interplay between reactive and intermediate molecules and the electrode surface at the microscopic level is essential for advancing our understanding of (electro)catalysis. These interactions have profound implications for the overall catalytic activity of materials, operating at the mesoscopic level. In this sense, microkinetic modelling is a powerful approach that bridges these two levels by unravelling the global kinetics of a reaction from the contribution of each individual step within the reaction mechanism. Here, we present a systematic methodology for constructing a robust microkinetic model, encompassing four crucial stages: (i) gathering information and mechanism statement, (ii) model establishment, (iii) numerical simulations,
and (iv) comparison with experiments. To demonstrate the efficacy of this methodology, we applied it to investigate the mechanisms governing the electrooxidation reactions of formic acid and methanol. In the final stage of the methodology, experiments under oscillatory dynamics proved to be a remarkably sensitive tool for model validation. Compared to traditional techniques such as cyclic voltammetry (CV) and chronoamperometry (CA), these experiments exhibited superior sensitivity to changes in the reaction mechanism and rate constants for each elementary step. Furthermore, we conducted a sensitivity analysis on our models, quantifying

the individual contributions of each reaction step within the electrocatalytic system towards the overall oscillatory response. This comprehensive approach not only enhances our understanding of (electro)catalytic processes at the microscopic level but also paves the way for the development of materials with greatly improved catalytic properties.

Keywords: Methanol electro-oxidation, formic acid electro-oxidation, microkinetic modelling, oscillations, numerical simulations.

Introduction and Objectives: A thorough understanding of the intricate interplay between reactive and intermediate molecules and the electrode surface at the microscopic level is essential for advancing our understanding of (electro)catalysis. These interactions have profound implications for the overall catalytic activity of materials, operating at the mesoscopic level. In this context, microkinetic modelling emerges as a powerful approach, bridging the gap between these two levels by unravelling the global kinetics of a reaction through a meticulous examination of each individual step within the reaction mechanism. Here, our goal is to introduce a systematic methodology for building a robust microkinetic model.

Methodology: The construction of a microkinetic model encompassing four crucial stages:

(i) gathering information and mechanism statement,
(ii) model establishment,
(iii) numerical simulations,
(iv) validation through experimental comparisons.

To demonstrate the efficacy of this methodology, we applied it to investigate the mechanisms governing the electrooxidation reactions of formic acid and methanol.

Preliminary results: Experiments under oscillatory regime proved to be more sensitive for model validation compared to traditional techniques such as cyclic voltammetry (CV) and chronoamperometry (CA), as they showed superior sensitivity to changes in the reaction mechanism and rate constants for each elementary step.

Preliminary conclusions: This approach improves our understanding of (electro)catalytic processes at the microscopic level by evaluating the kinetic response at the mesoscopic level, paving the way for the development of materials with greatly improved catalytic properties.

Fátima Eduarda do Nascimento Morais
USP

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Abstract Title: Methods for the analysis of resonance in distribution systems with high DER penetration

Authors' Names & Affiliation Institutions of all authors (in order for publication):
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Abstract:
The Brazilian energy sector has undergone an intense modernization to improve its generation capacity. In recent years, the participation of hydroelectric plants in energy dispatch has decreased due to the increased penetration of distributed energy resources. Consumers who used to be passive are now active generators and managers of their energy. With this growing demand on the distribution network, capacitor banks are used for voltage control and power factor improvement, and the complexity of network operation has increased. Depending on the operating conditions and network topology, the interaction between these devices can cause resonance. In addition to causing problems in the power generation system, resonances are also a concern for electricity distribution companies. The Brazilian energy sector is concerned about resonance phenomena and how they can negatively influence distribution networks. With this issue in mind, the project aims to develop four models for analysing resonances in distribution networks connected to a storage system, two of which are detailed models in the time domain for medium and low voltage, and two are simplified models in the frequency domain for medium and low voltage. The simplified model will then be compared with the detailed model to verify if it meets the requirements for efficiently identifying resonances for use in studies to mitigate this issue.

Keywords: Generation, Resonances, Models.

Introduction and Objectives: Due to the growing changes in the Brazilian electricity sector, there has been a reduction in the reservoirs' regulation capacity and, consequently, a decrease in the use of thermoelectric power plants, which has made it necessary to diversify the Brazilian energy matrix safely and cleanly to meet the population's needs. Integrating these resources directly into the grid can lead to issues such as violating medium and low-voltage operating constraints and system protection failures, among others. Still, the problem that raises the most concern is the increase in resonant phenomena. Resonances occur in distribution feeders compensated by capacitor banks, as these are designed to facilitate voltage support and improve power factor, especially in scenarios where a DER (Distributed Energy Resource) is inserted. To efficiently identify resonances, this project aims to create four models: two in the time domain for medium and low voltage, in which a detailed model will be developed and simulated using Matlab Simulink to simulate these models, and two simplified models in the frequency domain. A comparison will be made between the detailed and simplified models to verify if the new frequency domain model meets the criteria for identifying resonances that may exist in a

distribution system with DERs practically and efficiently. The secondary objectives of the research project are:

● To carry out bibliographical studies on resonances and their characteristics;

● To create a detailed time-domain model for identifying resonances in medium and low-voltage energy storage systems;

● Simulate the detailed model in MATLAB Simulink;

● Create a simplified model in the frequency domain to identify resonances in an energy storage system for medium and low voltage;

● Simulate the simplified model in OpenDSS;

● Comparing the detailed time-domain model with the simplified frequency-domain model and making possible improvements to the model.

Methodology: The methodology of this project involves investigating resonance phenomena and their critical scenarios in DER parameters to carry out detailed modelling in the time domain using MATLAB Simulink to simulate the model. Next, a new, more simplified model will be made, but this one will be in the frequency domain, using the OpenDSS simulation software that allows for the frequency domain model. Finally, the last stage consists of comparing the two models to check whether the simplified model serves the purpose of verifying systems that present resonances.

Preliminary results: This project does not yet have results to describe, as it is still in the literature review phase, to understand what resonances are and how they can impact the Brazilian energy sector.

Preliminary conclusions: As the project is still in the bibliographical research phase, it is not yet possible to draw any positive or negative conclusions about the proposed project

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Abstract Title: Catalysts for hydrogen production in ethanol-fed SOEC systems

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Abstract: In this work different catalysts were developed to operate in the anode/cathode of solid oxide electrolytic cell, to perform the ethanol electrochemical reform for hydrogen

production at a temperature of 800°C. In this system, ethanol is used as fuel to reduce the amount of electrical energy spent in the process. The cells were built with the LSGM (Lanthanum Strontium Gadolinium Manganesium Oxide) electrolyte, having the developed materials mixed with GCO as catalysts in both, the cathodic and anodic layers. For LSMN (Lanthanum strontium manganite doped with Nickel Oxide), LSCN (Lanthanum strontium cobaltite doped with Nickel Oxide), LSZN (Lanthanum strontium zincate doped with Nickel Oxide), LSCuN (Lanthanum strontium cuprate doped with Nickel Oxide) and LSFN (Lanthanum strontium ferrite doped with Nickel Oxide) at 1000 °C, XRD results confirm the peroviskite structure of the prepared catalysts, but with the presence of minor multiple signals referring to different segregated oxide structures, specially SrO2 and NiO. Electrochemical experiments show that the performance of the cell operating with ethanol in the anode was notably superior to that operating with air, in which case the reaction is the oxidation the O2- species crossing the electrolyte, instead of ethanol.
Analyses of the anode exhaust evidenced formation of large amounts of hydrogen, CO, methane, ethane and ethylene, possibly coming of the ethanol oxidation, but also from parallel occurrence of ethanol chemical reform. On the cathode exhaust, it is seen the presence of hydrogen with some quantity of carbon monoxide, methane, ethylene and ethane impurities that reaches the cathode after crossing the electrolyte layer.

Keywords: Hydrogen production; Solid oxide electrolytic cell; Cell supported on the electrolyte.

Introduction and Objectives: Minimizing dependence on petroleum derivatives to produce energy has become decisive for the sustainable development of any society, and in this scenario, the generation of clean energy from renewable sources has brought new scientific and technological challenges. Among the various alternatives, hydrogen has attracted much attention for generating energy without the release of polluting substances. In this context, solid oxide electrolytic cells (SOEC) can be used to produce green hydrogen from water reduction and biofuels oxidation, particularly ethanol and glycerol.

The objective of this work was of developing catalysts for hydrogen production in solid oxide electrolytic cells. Synthesized materials comprised LSMN (Lanthanum strontium manganite doped with Nickel Oxide), LSCN (Lanthanum strontium cobaltite doped with Nickel Oxide), LSZN (Lanthanum strontium zincate doped with Nickel Oxide), LSCuN (Lanthanum strontium cuprate doped with Nickel Oxide) and LSFN (Lanthanum strontium ferrite doped with Nickel Oxide). The catalysts are used at the anode/cathode for cell construction, having LSGM (Lanthanum gallate, strontium and magnesium doped) as electrolyte.

Methodology: The activities involved first the preparation of LSMN, LSCN, LSZN, LSCuN and LSFN materials and their evaluation for the catalytic activity for fuel oxidation and hydrogen evolution reactions in water electrolysers. These materials were prepared via Pechinni method with all salts solubilized in aqueous citric acid solutions. These solutions were boiled and then ethylene glycol was added into the system, which was next heated until 135°C for gel

formation. The material was thermally treated at 500°C for 2 hours, followed by 1000°C for three hours. Specifically, for the LSCN catalyst, heat treatments were conducted at 500°C, 650°C, 750°C, 1000°C, 1100°C and 1300°C. The characterization of produced materials were made by X-ray diffraction (XRD), for analysing their crystallinity and structure.
The single SOE cells were prepared in the form of pellets containing the anode, electrolyte, and cathode. As a first step LSGM electrolyte pellets (1.5 mm thick, 2 cm2 geometric area) were prepared by pressing the precursor powder, followed by thermal treatment at 1350°C in air for 12 hours. The catalysts were first mixed with GCO (Gadolinium Cerium oxide) and then deposited as films in both faces (5 mg cm-2) of the electrolyte pellets, by brushing a suspension of these composites in a isopropanol and terpineol mixture. After depositions, the cell pellets were subjected to a heat treatment at a temperature of 1000°C for 2 hours to sinter the catalytic layers and firmly stick them to the electrolyte. The single cells electrochemical experiments were conducted using a potentiostat, with the SOEC sealed inside a ceramic tube and fed with humidified Ar/ethanol into the anode and water introduced into the cathode. The experiments were carried out in an oven at a temperature of 800°C. The electrochemical experiments involved polarization and electrochemical impedance spectroscopy measurements to analyse the performance and integrity of the systems. The products of water reduction and ethanol oxidation were monitored by gas chromatography.

Preliminary results: For LSMN (Lanthanum strontium manganite doped with Nickel Oxide), LSCN (Lanthanum strontium cobaltite doped with Nickel Oxide), LSZN (Lanthanum strontium zincate doped with Nickel Oxide), LSCuN (Lanthanum strontium cuprate doped with Nickel Oxide) and LSFN (Lanthanum strontium ferrite doped with Nickel Oxide) at 1000 °C, the X-ray diffraction results evidenced peaks around 33°, 43°, 47°, 57°, 67°, 78° and 95° that confirm the perovskite structure of the prepared catalysts. However, results also indicate the presence of minor multiple signals referring to the presence of different segregated oxide structures, specially SrO2 (peak at 31.9°) and NiO (peaks at 42.4° and 44°). XRD analyses of the LSCN catalyst prepared at different temperatures showed that the perovskite phase is produced above 650°C. In this lower temperature only minor formation of segregated of NiO is detected, while the presence of SrO2 is evidenced above a heat treatment temperature of 750°C. In both cases, the amounts of segregated phases increase a little with the increase of temperature. Polarization measurements conducted for the SOEC with the LSCN catalyst in the anode and cathode, for systems with ethanol or air fed to the anodic compartment and water to the cathode. Results show that the performance of the cell operating with ethanol in the anode was notably superior to that operating with air, in which case the reaction is the oxidation O2- species crossing the electrolyte, instead of ethanol. In fact, chronopotentiometric results showed that at 0.6 A cm-2 the cell fed with ethanol operates at voltages around 0.6 V, while when exposed to air the voltage is 1.5 V in the same current density. Impedance results obtained for the cell fed with ethanol at the open circuit potential evidence a quite small charge transfer resistance (close to 1 Ω cm2), confirming the high performance the SOEC for producing hydrogen when ethanol is oxidized at the anode. A comparison of the performances of the LSCN and LSMN cells fed with ethanol in the anode shows that the LSCN catalyst presents greater activity compared to

that of LSMN. The most probable cause for this effect may be assigned to the difference in the intrinsic activity of the catalysts to promote the fuel oxidation and/or water reduction reactions. Gas chromatographic analyses of the anode exhaust showed formation of large amounts of hydrogen, carbon monoxide, methane, ethane and ethylene, this evidencing parallel occurrence of the ethanol chemical reform, as promoted by the investigated catalysts. On the other hand, analyses of the cathode exhaust confirmed the presence of hydrogen, but with some quantity of carbon monoxide, methane, ethylene and ethane. In this case, these impurities possibly come from the crossover of gases from the anode to the cathode.

Preliminary conclusions: For all the materials, the peroviskite structure were confirmed, but with the presence of different segregated oxide structures, specially SrO2 and NiO. Electrochemical experiments showed that the performance of the cell operating with ethanol in the anode was notably superior to that operating with air. Analyses of the anode exhaust evidenced formation of large amounts of hydrogen, CO, methane, ethane and ethylene, possibly coming of the ethanol oxidation, but also from parallel occurrence of ethanol chemical reform. On the cathode exhaust, it is seen the presence of hydrogen with some quantity of carbon monoxide, methane, ethylene and ethane impurities that reaches the cathode after crossing the electrolyte layer.

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Abstract Title: Methods for analysis and mitigation of resonances in DER-rich distribution systems

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Paulo – USP).

Abstract: Modern electrical energy distribution systems are experiencing significant changes, especially with the rapidly increasing penetration of distributed energy resources (DERs), such as photovoltaic and wind generators, electrical vehicles, and energy storage systems. These devices use power electronic-based technologies, which may present negative resistance characteristics at specific frequencies. Therefore, these power electronic-based DERs have the potential to decrease resonance damping in the electrical system and, consequently, damage circuit equipment and customer loads (customer processes). This can create significant financial losses not only to the distribution utility, but also to the end customer. As the high penetration of DERs in distribution systems is a relatively recent trend, it remains unclear which are the main characteristics and most critical scenarios of these resonances. In addition, there are no well-established methods to anticipate the risk of these problematic resonances and mitigate them. In this context, the goal of this project is to provide a detailed characterization of these resonances in DER rich distribution systems and develop methods to predict the risk of occurrence of these resonances and mitigate this risk, avoiding costly damages to circuit equipment. The focus is on the development of systematic methods that can speed-up the decision-making process of engineers in terms of which actions should be undertaken to avoid or eliminate resonances, either during planning or operation of DER-rich distribution systems. The results of this project will be used not only to reduce the risks and costs associated with technical losses and device damages, unplanned disconnection of customer processes, equipment lifetime reduction, and number of man-hours needed to manage these resonances. The results of this project can also be used to support the improvement of national regulations for DER integration into the distribution systems.

Keywords: resonance; distributed energy resources; DER; capacitor; mitigation; prediction; power electronic converters.

Introduction and Objectives: Recently, electric power distribution systems have migrated from a passive, non-supervised structure with low level of automation to an active, supervised structure with high level of automation due to the introduction of DERs and new automatic control devices. The most common DERs include wind turbines, electric vehicles chargers, energy storage systems and, primarily, photovoltaic generators. In Brazil, it is estimated that PV generation will account for over 97% of the distributed generation capacity installed over the next decade. A common characteristic of these DERs is that they have a power electronic converter as their interface with the grid.

In terms of new utility devices installed in the system, in the context of this work, it is important to highlight automatically operated capacitor banks, which can be installed at Medium Voltage (MV) grids, as usual, or even be installed dispersedly over the system at the Low Voltage (LV) grids, and a more frequent installation of switched series capacitor banks to supply loads or distributed generation at locations far from the substation.

The increased presence of shunt and series capacitors combined with the increased presence of

power electronic-based DERs has the potential to increase the amount and severity of resonances in the circuit. The reason is that the power electronic converters used in DERs (mainly the voltage source converters) can have a negative resistance characteristic at specific frequencies. If a negative equivalent resistance matches a resonance frequency in the circuit, the resulting effect is that resonance damping will decrease (creating weakly damped resonances) and potentially become negative (creating unstable resonances), which can damage circuit equipment and create significant financial losses to the distribution utility and to the customers. This effect can happen both at LV systems, where shunt capacitors are being installed, and at MV systems, where shunt and series capacitors are installed.

One challenge with this scenario is that distribution utility engineers are not traditionally concerned with weakly damped resonances and instabilities and tend to address them on a case-by-case basis, which are normally based on numerous detailed electromagnetic transient or frequency-domain simulations. However, with the increased penetration of DERs, such events are bound to become more frequent. Hence, it is essential to investigate and develop new approaches to systematically manage the risk of these events without the need to run time-consuming computer simulations.

The main objective of this research is to investigate the characteristics of resonances in power distribution systems with high penetration of DERs and develop practical methods for managing (anticipating and mitigating) the risk of these events.

Methodology: Two main types of resonances will be investigated: resonances on LV distribution systems and resonances on MV distribution systems. More specifically, LV systems are smaller, and the predominant inductance is from the distribution transformer (line inductances can be neglected in most cases), whereas MV systems are larger, and the line inductance is significant. Adverse events on LV systems affect a few tens of customers, whereas an equivalent event on MV systems affects thousands of customers. DERs installed in LV systems are mostly single-phase devices (although some three-phase devices may also exist), whereas DERs installed in MV systems are three-phase devices. These different characteristics highlight that the behavior of resonances on LV systems is expected to be different (different root causes, different participation factors of the DERs, different mitigation approaches etc.) from the behavior of resonances on MV systems.

For each type of resonance, the following specific objectives can be outlined:

- Characterization: investigate and identify the main causes of the event and the critical scenarios where it can be initiated, which consists in identifying the parameters of the DER and of the power system with highest impact on the risk of resonance;

- Detection of the risk of occurrence: develop methodologies for the expedited and systematic identification of the risk of resonance in distribution systems, based on the characteristics (topological and operational) of the circuit;

- Mitigation of the risk of occurrence: develop methodologies to mitigate the risk of resonance in a distribution circuit (avoiding the onset of an event), or to mitigate already ongoing resonances; and - Power-Hardware In the Loop Simulations to evaluate the methods developed.

The knowledge obtained during this research and the methodologies developed will create the technical basis to support potential improvements on the national regulation about the integration of DERs.

Preliminary results: As the project is in its early stages, there is no preliminary results.

Preliminary conclusions: As the project is in its early stages, there is no preliminary conclusions.


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Chairs: Cristina Fernanda Alves Rodrigues – Pedro Vidinha

Ana Carolina Borges Silva
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Abstract Title: Particle resolved CFD simulations of fixed bed reactors in co2 hydrogenation

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Abstract: In recent years, CO2 hydrogenation has gained significant attention as a promising method for carbon capture and utilization. Particle Resolved Computational Fluid Dynamics (CFD-PR) simulations is a powerful approach to study and optimize chemical reactions and processes involving multiphase systems, since it provides detailed insights into fixed-bed reactors. This approach also offers a comprehensive platform to investigate the complex interaction between particles, fluids, and chemical reactions in these systems using modelling techniques to capture the behaviour of individual particles, such as catalyst particles, within the fluid flow, being capable to provide detailed information on particle dynamics, enabling a deeper understanding of the reaction mechanism and catalyst performance. Highly exothermic heterogeneous catalytic reactions are performed commonly in fixed-bed reactors, being necessary an adequate modelling that can be carried out with full computational fluid dynamics (CFD). CFD simulations were performed with a relation between the reactor diameter and catalyst particle diameter of D/dB >10, in the transient flow regime and the random fixed bed is generated with a DEM-code. The focus of this work was to verify if the spatially resolved randomly distributed particles allows a comprehensive description of the interstitial flow, capturing detailed particle behaviour and fluid dynamics, offering valuable insights for process optimization and the development of sustainable carbon capture and utilization strategies.

Keywords: Particle-Resolved CFD, fixed-bed reactors, CO2 hydrogenation.

Introduction and Objectives: Under development.
Methodology: Under development.
Preliminary results: Under development.
Preliminary conclusions: Under development.

Priscilla J Zambiazi
University of São Paulo

Abstract Title: Engineering porous materials MOFs-Based - Technological Applications and Dynamic Crystals.

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Abstract: MOFs (Metal-Organic Framework structures) are notorious materials with unique properties due to their three-dimensional network structure and crystalline dynamism. To fully exploit their practical potential, multifaceted structural studies are essential for comprehending their physical and chemical properties linked to the crystallographic effect of their porous network. This research aims to drive innovative applications in social and economic development. In this work, we explore the properties of the crystal and molecular structure to develop new coordination polymers based on metal centres linked by polydentate anions, which bind through more than one atom to multiple metal centres. We investigate the solution chemistry, reactivity, physical properties, and the determination of the solid-state structure of the new complexes. Our initial focus centres on the crystallization of the new complexes, culminating in the formation of solid structures that reflect the binding process, ultimately yielding new supramolecular materials. These materials exhibit beneficial physical and electronic properties, including magnetism, porosity, and dynamic crystals, offering an efficient avenue for optimizing highly ordered porous networks with diverse applications in molecule capture and delivery.

Keywords: Metal-Organic Framework, Gases Capture, Nutrients release, Crystal Dynamics, Porous Materials Engineering.

Introduction and Objectives: The development of open structures constructed by atoms or clusters of metals interconnected by organic ligands has attracted significant interest, primarily due to their potential for various applications, such as gas storage, separation, catalysis, controlled nutrient delivery, among others. These structures have numerous unique structural characteristics. Structures with flexible yet stable architectures may serve as hosts for various reversible dynamic processes triggered by external stimuli. Some structures can intelligently adjust their porosities to accommodate guest molecules, going through retraction, expanding, and/or distortion. These structures occupy a middle ground between rigid metal coordination structures and highly flexible self-assembled materials based on supramolecular interactions. The key advantage of flexible structures is that their crystallinity is maintained after modification, enabling structural studied that can subsequently fine-tune various properties, including magnetic, resulting in a wide range of multifunctional materials. Coordination

polymers fall within the broad concept of supramolecule by using intermolecular bonds as a self-assembly to control the packing within crystalline solids, thereby imparting specific properties to these materials. This class of materials applies the term “crystal engineering” to describe the supramolecular process responsible for controlling crystal architecture. Thus, coordination polymers that connected in 3D with microporosity are referred to as MOFs. The metal-ligand networks constructed feature metal nodes forming a 1D arrangement known as SBUs, which are essential for achieving MOF porosity, and are increase to 3D by organic linkers bridging. Most studies on MOFs focus on creating robust structures, emphasizing their capacity to preserve their architecture even after the removal of host solvent molecules for practical applications. MOFs exhibit remarkable versatility as they undergo single-crystal to single-crystal transition triggered by external stimuli. Recent attention has focused on porous solids formed by MOFs. Donor groups such as N, carboxylates, sulfonates, or imidazolates facilitate bonding between the organic component and the metal center. The advantage of this process is that pore size can be easily controlled. For example, Yaghi et al created cubic cages based on the Zn metal center linked by 1,4- benzenecarboxylate or similar groups. The volumes within these cages can be range from 1100Å3 to 12000Å3. These porous solids were utilized to absorb gases such as H2, N2, and Ar. More recently, they have been employed to store CO2 and show promise in delivering nutrients hosted within their pores. This study aims to produce MOFs with useful properties, such as magnetism, high surface area, and adjustable porosity. For instance, current laboratory work involves Fe(II/III)-MOF that are similar to those used for controlled nutrient release.

Methodology: The materials proposed in this study were synthesized via hydrothermal methods using water as a solvent and were subjected to investigation through by single-crystal X-ray diffraction and Mössbauer spectroscopy. These techniques offer an efficient approach to optimizing highly ordered porous networks, with the goal of producing crystalline solids capable of exhibiting solid-state dynamics.

Preliminary results: The crystal structures of MOFs are being analysed as host molecules change in addition to controlled nutrient delivery. The resulting compounds find applications as “new materials” in the solid state, offering valuable properties suitable for advanced and innovative technologies.

Preliminary conclusions: The results obtained in this study hold practical applications across the production chain, including the storage of gases like CO2, ammonia, and hydrogen, also other molecules as well as water. The flexible polymeric structure enables deformation of the solid to facilitate the entry of small gases under pressure and the delivery of small molecules, expanding the field of applications.

Andressa Mota-Lima
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Abstract Title: Assessment of Non-Aqueous Electrolytes for CO2 Electro-reduction via updated Walden Plot

Authors' Names & Affiliation Institutions of all authors (in order for publication): Andressa Mota-Lima (EP-USP/DEQ) and Claudio Augusto Oller do Nascimento (EP-USP/DEQ)

Abstract: Electroreduction of CO2 represents the electrification of the life cycle of the CO2 molecule and can serve as a technology within the portfolio of a carbon capture and utilization-based economy. In this critical assessment, the grounds of Wade Plot are revised under the light of the most up-to-date available data on the intrinsic ionic conductivity of non-aqueous electrolytes. The updated Walden Plot method is utilized to analyse the relationship between the conductivity and viscosity of the electrolytes, providing a graphic method for selecting suitable electrolytes for CO2 electro-reduction reactions. This assessment helps in identifying and selecting the most suitable non-aqueous electrolytes for CO2 electrochemical conversion processes.

Keywords: CO2 Electrochemical conversion processes, updated Wade Plot, Ionic Liquids, non-aqueous electrolytes, conductivity and viscosity.

Introduction and Objectives: Electrochemical reduction of CO2 (CO2RR) has been part of the technological solution for the long-term anthropogenic effects of greenhouse gasses. Ordinarily, CO2RR is carried out in water, however, even carbonate-contained water is far from being a good solvent for CO2. In this context, the search for a solvent that could be both used as CO2-absorbed and CO2R-electrolyte has been raised as a good path to pave marketable products. Herein, we survey physical-chemical properties of electrolytes for electrocatalysis with potential use as CO2 absorbents.

Methodology: A survey on the scientific data on molar conductivity, viscosity and density of pure substances are conducted. Eventually for those pure substances that are not conductive, we considered salt, acid or base containing substances. Most of the information about organic and inorganic substances was appropriately compiled by prof. Roger Parson in the book named Handbook of Electrochemical Constants, being them used in this present work. On the other hand, data on ionic liquids was collected from most up-to-date publications.

Preliminary results: The update Walden plot elucidates that either liquid ammonia or hydrazine are good electrolytes for electrocatalysis in terms of both appropriate electrical conduction and low viscosity. However, hydrazine must be overlooked given its corrosive properties and explosion risk.
Compared to high pressure water electrocatalysis, the high-pressure liquid ammonia

electrocatalysis has a vapor liquid equilibrium favouring the ammonia vapor. As a result, we expect a larger loss of electrolyte toward ammonia vapor than the loss observed when water is used as electrolyte. On the other hand, liquid ammonia also has potential to be an electrolyte in the plasma electrolysis configuration, even though its narrowed thermodynamic stability as liquid at atmospheric pressure. At pressure equal 1 atm, ammonia must be below -33 °C in order of being in liquid form.

Preliminary conclusions: Liquid ammonia has potential to be used in the CO2 electroreduction reaction given a combination of factors: (1) both appropriate electrical conduction and low viscosity, and (2) potential to absorb CO2 at large extent given the high pressure-induced carbamate formation, a organic group formed between the unpaired electron pair in ammonia and the carbon dioxide molecule.

Bryan Alberto Laura Larico
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Abstract Title: Development of a technical catalyst for the conversion of CO2 into methanol

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Abstract: The use of catalysts is crucial for the production of various chemical products, making large-scale production possible or even the possibility of producing products that were previously obtained by unconventional means. As a result, the field of catalysis has received significant attention due to the potential for converting CO2 into other products, such as methanol. The incentive for CO2 conversion arises from the large production of this gas from petroleum, coal, and natural gas in recent years,
leading to an increase in the greenhouse effect. There are numerous challenges in CO2 conversion, with the most significant being its high thermodynamic stability. However, there are already various catalysts for the conversion of CO2 into numerous products, but the widespread use of CO2 for chemical production is still limited. The largest usage is in an industrial plant in Iceland, which consumes about 5,500 tons/year of CO2, representing a very

small fraction compared to global emissions. From this perspective, the work aims to develop a technical catalyst (pellet) for the conversion of CO2 into methanol under high pressure on a semi-industrial scale. Preliminary results show that there are a series of factors that affect the pellets, and it is still a relatively unexplored field in academia.

Keywords: CO2, methanol, technical catalyst, rhenium.

Introduction and Objectives: The use of catalysts in the production of chemical products has become almost a rule in the industry, acting directly or indirectly in the production of about 90% of current chemical products. In other words, there is extensive use of materials with catalytic action.

As a result of this significant presence in the manufacturing of products, the catalysis market generates billions of dollars every year, continuously growing. This financial activity is also justified by the great versatility of catalysis, which generally facilitates or even makes possible the formation of a specific product, and it is identified according to the principles of green chemistry.

With this theme, catalysis has received worldwide attention as a possible tool for CO2 reduction. CO2 emissions from petroleum, coal, and gas have been increasing each year, being one of the main greenhouse gases. Data from "Our World in Data" show that since the last century, CO2 emissions increased from 5 gigatons (Gt) in 1950 to 35 Gt in 2018. This rapid growth in CO2 emissions is directly related to the growing energy demand.

One of the significant challenges involving the transformation of carbon dioxide molecules is their high thermodynamic stability, with a Gibbs free energy of -394 kJ/mol, making this molecule less utilized, often being a byproduct of various reactions, such as petroleum cracking, hydrocarbon combustion, and others.

From these perspectives, the conversion of CO2 into higher-value products is a scientific challenge, and scaling it up for large-scale production of CO2-derived products is a significant technological challenge. However, there has been considerable progress in the production of CO2 into methanol, with the implementation of an industrial methanol production plant in Iceland, the George Olah plant, converting 5,500 tons/year of CO2.

Despite the operation of an industrial CO2-to-methanol conversion plant, there is still a significant gap in the academic community in understanding the scale-up process. Among some of the reasons for this are the lack of project funding, industrial interests, numerous patents, and the interdisciplinary nature of the field.

With that said, among the objectives of this work are the construction of rhenium oxide pellets on titania, CO2 conversion into methanol under high pressure on a mini-pilot scale using rhenium oxide catalyst in pellet form, and characterization of the pellets through XRD, TGA, TPR, TPO, and other techniques.

Methodology: Titanium dioxide pellets were synthesized using different additives for the paste used in extrusion. Among the additives used were polyvinyl alcohol (PVA) 98% hydrolysed, acetic acid, carboxymethyl cellulose, and hydroxymethyl cellulose. After extrusion

of the pastes, the pellets were calcined at temperatures of 400°C and 600°C. The impregnation of rhenium was carried out after the calcination of the pellets, and the method used was aqueous impregnation using the ammonium perrhenate precursor. In conjunction with the synthesis of the materials, various characterizations were necessary. These included the use of X-ray diffraction (XRD) to determine crystalline phases and crystallite size, determination of surface area and porosity through nitrogen physisorption measurements, temperature programmed reduction (TPR) using H2 to determine the reduction temperatures of the materials, and thermogravimetry (TGA) to determine the temperatures at which chemical transformations occurred. Atomic emission spectrometry by inductively coupled plasma (ICP-OES) analysis was performed to determine the active metal content in the pellet.
Finally, catalytic tests were conducted on a mini-pilot scale, which had 10% of the capacity of the pilot plant. 1.2 grams of pelletized catalyst were used for the reactions. A gas chromatography system was coupled to the reactor to determine the conversion and selectivity of the catalyst.

Preliminary results: Preliminary analyses have shown that after calcination at 600°C of the titanium dioxide pellets, there is a phase transformation from anatase to rutile, along with crystallite growth. Additionally, ICP analyses have revealed a loss of rhenium when it is impregnated before calcination, with a 50% metal loss after calcination at 600°C for 4 hours and a 20% metal loss after calcination at 400°C for 4 hours. This led to the decision to use the impregnation method after calcination to avoid metal losses. These analyses were conducted for the pellet sample containing the PVA and acetic acid additives, and further analyses are required for the characterization of the cellulose pellets. Catalytic tests have shown some activity of the pelletized catalysts, but further refinements are needed to increase CO2 conversion and methanol selectivity.

Preliminary conclusions: The construction of pellets is still a relatively unexplored field, with limited available material in the literature. Therefore, a study of the impact of each additive on the catalytic step is a significant challenge. That said, further studies are being conducted to understand the correlation between conversion and selectivity with the preparation of the pellets.

Alberto Torres Riera Junior
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Abstract Title: Lattice Boltzmann methods applied to the solution of Digital Rock problems

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Abstract: The characterisation and comprehension of fluid dynamics within porous mediums are important in geochemical processes. This is especially pertinent to the petroleum industry, where grasping and forecasting the interplay between porosity and permeability is pivotal, particularly at the microscopic
pore scale and its integration with reservoir simulations. Lattice Boltzmann (LB) methods offer a means to delve into and incorporate microscopic mechanisms at the pore level. Yet, it remains a challenge to encompass various underlying physical-chemical phenomena and to replicate the morphologies and geometries inherent in realistic porous media akin to those found in digital representations of rocks. In this work, we aim to compare and validate different LB methods for simulating the flow of oil-water mixtures in digital rocks at the pore level.

Keywords: Lattice Boltzmann, Digital Rock, Enhanced Oil Recovery.

Introduction and Objectives: The characterisation and comprehension of fluid dynamics within porous mediums are important in geochemical processes. This is especially pertinent to the petroleum industry, where grasping and forecasting the interplay between porosity and permeability is pivotal, particularly at the microscopic pore scale and its integration with reservoir simulations. Lattice Boltzmann (LB) methods offer a means to delve into and incorporate microscopic mechanisms at the pore level. Yet, it remains a challenge to encompass various underlying physical-chemical phenomena and to replicate the morphologies and geometries inherent in realistic porous media akin to those found in digital representations of rocks. The overarching objective of this project is to advance the field by developing and applying Lattice Boltzmann simulations in conjunction with digital rock models. This endeavour will involve enhancing the physical descriptions within the Lattice Boltzmann models. We'll do this by incorporating and rigorously validating factors such as wettability, heterogeneity, and boundary conditions. Establishing protocols for predicting relative permeability in digital rock models is particularly important while considering different Lattice Boltzmann techniques.

This proposal also seeks to bridge a gap in fundamental knowledge by refining our understanding of fluid-fluid and fluid-rock interactions via molecular modelling. Simultaneously, we will create tools to integrate LBM with it seamlessly) machine learning techniques, and ii) scientific visualisation tools using interactive virtual reality. Drawing upon the knowledge amassed throughout this project and its integration with digital rock models, we will conduct computational experiments involving the injection and immiscible two-phase flow within porous media. Our specific goals include estimating the oil recovery factor under varying thermodynamic conditions and scenarios: i) injection of different fluids (including aqueous solutions of nanoparticles, surfactants, and low-salinity brine) for the displacement of oil, and ii) assessing the material types and pore geometries in the rocks of interest, utilising digital rock models and empirical data. The anticipated outcomes of this project will not only facilitate the

mapping of Lattice Boltzmann implementations and validation processes but also enhance the predictive capabilities of these methodologies. Furthermore, this research will contribute significantly to the understanding, characterisation, and optimising enhanced oil recovery techniques (EOR) employing digital rock models.

Methodology: To accomplish the goals of this project, we are going to employ Lattice Boltzmann methods such as the colour-gradient [Physical Review A 43, 4320 (1991)] and pseudo-potential with explicit forces [Physical Review E 65, 046308 (2002)] LB models.
The color-gradient Lattice Boltzmann (LB) method introduces two velocity distribution functions to characterise distinct fluids. Additionally, a perturbation operator based on colour gradients creates surface tension effects. This operator also includes a recolouring step, which aids in the separation of various phases or components.
Within the explicit force pseudo-potential model, fluid interactions are mimicked by an interparticle potential that describes the nonlocal particle interactions, through which the separation of different phases or components can be achieved naturally.
The code packages Palabos (https://gitlab.com/unigespc/palabos), LBPM (https://github.com/OPM/LBPM), and Grad-LBM (a closed-source code authored by Diogo Nardelli Siebert and Rodrigo Surmas) will be used to run the simulations.

Preliminary results: To obtain the relative permeability versus saturation curves of a water-oil mixture at different water saturations, ranging from zero to one, Lattice Boltzmann simulations of the flow of that mixture have been performed with the code Grad-LBM, using the color-gradient model, periodic boundary conditions, and a constant pressure difference. Initially, two geometries were employed: a digital rock obtained from a CT scan of a standard synthesised silica beads sample and a parallel plate geometry. The simulations were run until a stationary state for the fluids' relative permeability and capillary number was reached. The results have shown a not well-understood behaviour of the relative permeability (krel) vs. saturation curves, displaying a non-expected decrease of the relative permeability of any of the fluids as they reach 100% saturation. This behaviour matches the simpler parallel plate geometry, ruling out any possible geometric effect. To identify and understand the cause behind this effect, several simulations testing different parameters have been performed: varying lattice resolutions; wettability (oil-wet to water-wet); pressure difference; the width of the liquid-liquid interface and diffusion in the model; and the interfacial tension.
A comparison using the same LB method (color-gradient) implemented in a different code (LBPM) and employing other LB methods (using Palabos) is being performed.

Preliminary conclusions: Although the colour-gradient LB model is a good choice for modelling dense fluids that are strongly immiscible, other Lattice Boltzmann methodologies, such as the pseudo-potential model with explicit forces, may be best suited to describe the liquid-liquid and solid-liquid interactions in a more physically sounded way.

Lais Reis Borges
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Abstract Title: Evaluation of intrinsic catalytic activity of rhenium catalysts at CO2 hydrogenation in a fixed bed reactor during a scale-up process

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Abstract: The rhenium-based catalysts are efficient for methanol synthesis trough CO2 hydrogenation process at low temperature (200°C) and high pressure (100 bar). The catalytic system developed at laboratory scale revealed the structure-activity relationship. The new project intends to scale up the methanol production to improve the process efficiency on a technical scale. For these, a technical catalyst will be formulated and shaped into pellets with an appropriate size, porosity and a high mechanical strength, chemical and thermal stability to avoid excessive pressure drops, minimizing the mass and heat transfer and maximize the access of fluid to active phase, as well as ensure a long lifetime. To implement this technology, the catalyst pellet efficiency had to evaluate with reliable experimental data and accurate intrinsic activities. The heterogeneous catalysis involves not only the chemical transformation on catalyst surface, but also the interphase and intraparticle diffusion of reactants to and products from and the adsorption of reagents and desorption of products from catalyst surface. Therefore, the intrinsic activity of a catalyst must be evaluated at conditions that the catalytic rate is not impacted by mass and heat transport. The operations parameters as reactor diameter, particle diameter and catalyst bed length should be selected carefully to ensure no limitation of mass and heat transfer during the evaluation of catalysts. The correlations of these parameters with catalytic activity of rhenium catalysts at CO2 hydrogenation will be studied.

Keywords: Scale-up, CO2 hydrogenation, catalytic performance, mass and heat transfer.

Introduction and Objectives: Methanol is commonly produced via synthesis gas (CO:H2), which is mainly obtained from fossil sources, from the reforming of natural gas or the gasification of coal. However, the synthesis of green methanol, produced via hydrogenation of CO2, is an interesting path and has been studied by many researchers in recent years due to the lower net carbon emission in this process. The main motivation for scaling the process of converting CO2 to methanol is the abatement and recycling of CO2, since based on the stoichiometry of the reaction and the conversion of 96% of carbon, for each ton of methanol, 1.43 tons of CO2 is used. When methanol is synthesized by the conventional process, the CO2 emission is 0.5-2.4 ton of CO2 per ton of methanol produced; in the other way, trough the production of methanol from CO2, emissions can be reduced by up to 90%, with emissions of around 0.2 t CO2/t methanol. The transformation of promising catalyst into a technical catalyst is not straightforward. The development of technical catalyst must optimize the mechanical resistance, reaction rate, mass transfer rate, reactor fluid dynamics and cost of production. The

additives as modifier, filler, binder, porogen, plasticizer, peptiser, lubricant, must be incorporated to powders to structure to enhance the properties and performance than research catalyst and structure the powders into mm-sized bodies. In addition to the in-depth characterization of the technical catalyst, the study of the reactivity and kinetic study of the events must be carried out under conditions in which there are no limitations on internal and external mass transport, and for this it must comply with some criteria, through the design of the factor effectiveness, Weisz-Prater number and sensitivity analysis. To avoid the diffusion limitation within the reactor, these criteria are directly related to physical parameters such as: reactor diameter must be at least 10 catalyst particle diameters and the catalyst bed length should be at least 50 particle diameters. Beyond, the experimental tests with variation of bed length and different ratio of particle diameter/reactor diameter must be carried out to ensure the operation of reaction in kinetic regime. To measure the intrinsic activity of catalyst, the mass transport intraphase/intraparticle must be controlled by modifying the geometric of pellet, effective thermal conductivity, and effective diffusivity. Furthermore, the exothermicity of CO2 hydrogenation can increment the temperature from external surface to center of particle, improving the reaction rate and changing the selectivity. Thus, a proper experimental condition had to be selected to absence of external and internal mass transport limitations, within an isothermally condition as possible. The dilution of catalyst bed with an inert material and a proper design of a reactor with a colling unit can guarantee a homogeneous temperature along the catalyst bed.

Methodology: The structured Rhenium based catalysts was synthesized via wet impregnation, with NH4Re2O4 precursor and commercially titania pellet of Saint Gobain (1.6 mm). This catalyst tested in flow reactor in CO2 hydrogenation (1CO2:4H2) at 200°C and 100 bar. The reactions parameters as bed length/ reactants flow, diameter of reactor and space velocity (20000 to 2500 ml g-1 h-1) will be performed with pellets catalysts.

Preliminary results: The initial results with pellets catalyst suggest that the rhenium catalysts in a powder form (particle diameter lower than 150 um) performed in a reactor with a diameter of ¼ in is not limitated by mass transfer. However, the pellets of 1.6 mm will be tested in different bed length/ reactants flow at same space velocity to verify the control of kinetics conditions.

Preliminary conclusions: The variation of particle diameter, reactor diameter and catalyst porosity affect the condition of mass transfer limitation.

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Abstract Title: NH3 Production via N2 electroreduction in Water-in-Salt Electrolyte with a MOF Catalyst

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Abstract: Electrocatalysis, presents a promising approach for NH3 production under ambient conditions, offering a sustainable alternative to the harsh conditions of Haber-Bosch process. The selection of both the catalytic material and electrolyte holds a crucial significance in achieving favorable outcomes in the electroreduction of N2 to NH3. In this work, the catalyst is based on metal-organic frameworks (MOFs) synergistically combined with metallic nanoparticles. The MOF selected, ZIF-8 (Zn-imidazolate), serves as a scaffold for hosting Ag nanoparticles, creating a hybrid material optimized for N2 electroreduction to NH3. Notably, this material possesses a water-blocking function, an important attribute to avoid hydrogen evolution reaction (HER). As electrolyte a unique water-in-salt electrolyte (WISE) was employed, which consists in lithium bis(trifluoromethanesulfonyl)imide salt (LiTFSI). In this electrolyte, the salt content surpasses that of water in both mass and volume. This approach serves to suppress the hydrogen evolution reaction (HER) and consequently fosters the generation of NH3. In our electrochemical studies, we employed Ag@ZIF-8 like catalyst, onto glass carbon electrodes. Controlled potential electrolysis was conducted to detect and quantify NH3. The NH3 detection and quantification were accomplished via Proton Nuclear Magnetic Resonance (1H-NMR), combined with a colorimetric method.

Keywords: Electrocatalysis, N2 Reduction, Metalorganic Framework (MOF), silver nanoparticles, Water-in-salt electrolyte, NH3 electrosynthesis, 1H-NMR detection.

Introduction and Objectives: The electrosynthesis of NH3 has gained significant attention in recent years. This is due to the fact that NH3 is produced by the Haber-Bosch process, which accounts for approximately 90% of global NH3 production. This process have several drawbacks since employes high temperature and pressure, which makes it highly cost. In addition, the other environmental problems are associated, such as the emission of greenhouse gases. Then, electrocatalysis offers an alternative option to produce NH3 under mild conditions compared to Haber-Bosch. As the HER is one of the challenges during the N2 reduction, the study of systems that suppress it have gained focus toward N2 electroreduction. Based on this, in this work, we employed ZIF-8 associated to Ag nanoparticles, creating a hybrid electrocatalytic material for N2 electroreduction. This material has a dual purpose, to act as an electrocatalyst and a water-blocking agent on the electrode surface. In addition, the selection of a WISE electrolyte has been another crucial aspect of our investigation.

Methodology:
Synthesis of Ag@ZIF-8
The Ag@ZIF-8 was synthesized via mechanochemistry, a solventless route. Initially, the metallic nanoparticles were synthesized over zinc oxide starting from the AgNO3 salt. Afterwards, the resulting material was milled with methyl imidazole resulting in the Ag@ZIF-8. The material was characterized by different techniques, such as, X-ray diffraction (XRD), inductively coupled plasma optical emission spectroscopy (ICP OES), scanning electron microscopy (SEM), and transmission electron microscopy (TEM).
Electrochemical Experiments
For the electrochemical experiments the material Ag@ZIF8 was deposited between in a glass carbon electrode by deep casting. Linear sweep voltametries were carried out under argon and N2 atmospheres using as electrolyte LiTFSI 15 mol kg-1 and 12 mol kg-1 in an single compartment electrochemical cell at 5 mV s-1. The controlled pulse electrolysis was carried out for 1h in N2 atmospheres at different concentrations of electrolyte. The NH3 detection and quantification were performed by colorimetric method and 1H NMR.

Preliminary results: The electrochemical profiles obtained by linear sweep voltametries under different atmospheres reveals that the Ag@ZIF-8 can catalytic reduce the N2 into NH3. The concentration of WISE demonstrated a significant role in the electrochemical profiles. Through controlled potential electrolysis under N2 atmosphere, was possible to produce NH3, which was detected and quantified by the colorimetric method and 1H NMR. The electrolysis at different concentrations of WISE shown that the production of NH3 is closely dependent of amount of water present in the system.

Preliminary conclusions: The catalyst synthesized, Ag@ZIF-8, is able to reduce electrochemically N2 into NH3 quenching the hydrogen evolution reaction. The amount of water in the system, plays an important role during the N2 reduction as observed for the different WISE concentrations. As the silver nanoparticles present the localized surface plasmon resonance (LSPR), further studies under laser irradiation can tune the ammonia electrosynthesis.

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Chairs: Renato Picelli – Fernando Sacomano

Enzo Sampronha
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Abstract Title: Modelling of Temperature-Swing Adsorption in Fluidized Bed Systems for CO2 Capture

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Abstract: The temperature-swing adsorption (TSA) process has been identified as a promising alternative for CO2 post-combustion capture due to relatively low cycle thermal energy consumption and because moderate temperatures and pressures may be applied. During the exothermic CO2 adsorption stage, heat is released in the process and during the desorption stage, by increasing bed temperature and applying a stripping gas, CO2 is desorbed and the adsorbent is regenerated. A possible way to improve the performance of TSA processes with respect to cycle duration, associated with bed heating and cooling times, is the use fluidized bed systems where gas-solid contact, and consequently heat and mass transfer phenomena, occur more intensely than in fixed beds. A semi-empirical approach based on the two-regions theory of fluidization (bubble and emulsion regions) is applied to modelling the controlling factors in a fluidized bed adsorption process. Single-stage simulation results show that gas-solid heat transfer is sufficiently high for gas and solids outlet temperatures to be practically equal, whereas the mass transfer from bubbles to emulsion is likely the most important resistance in a fluidized bed adsorber. In addition, greater CO2 recoveries lead to lower stage efficiency and CO2 selectivity.

Keywords: adsorption, fluidized bed, carbon capture.

Introduction and Objectives:
Introduction: The carbon dioxide (CO2) released due to the combustion of fossil fuels and organic matter has promoted the accumulation of this gas in the atmosphere, leading to several environmental problems related to climate change (Abanades et al., 2017). Post-combustion carbon capture processes are important for mitigating these emissions and, to this purpose, the use of solid adsorbents has been considered a promising technology due to lower energy consumption on sorbent regeneration compared to the conventional amine-based absorption process (Park et al., 2017).
The cyclic adsorption operation can be divided into adsorption and desorption stages. There are two fundamental adsorption cycle modes: Pressure Swing Adsorption (PSA) and Temperature Swing Adsorption (TSA). In a PSA cycle, adsorption and desorption occur under high and low pressure, respectively. In a TSA cycle, adsorption is conducted at low temperatures and desorption at high temperatures (Hedin et al., 2013). TSA technology is considered to be more practically applicable in continuous operation than PSA. Since continuously operating systems

are adequate for treating large flow rates of gas with relatively high CO2 content, continuous TSA carbon capture processes are a potential lower energy consumption alternative (Schony et al., 2017).
According to Zanco et al. (2018), due to limitations of fixed bed TSA CO2 capture, including: (i) heat transfer in bed heating and cooling, and (ii) large cross-sectional areas required to process high flow rates, recent studies have proposed circulating fluidized bed (CFB) systems as an alternative to traditional fixed beds. The fluidization regimes allow higher gas velocities and achieve greater heat and mass transfer rates compared to fixed beds (Kunii & Levenspiel, 1991), permitting a relatively precise bed temperature control. Also, CFBs can operate continuously as steady-state adsorption and desorption (regeneration) units. This work focuses on developing a model that captures the fundamental phenomena involved in the adsorption of CO2 in fluidized bed systems using TSA technology.

Objectives: To develop a mathematical model for fluidized bed adsorption of CO2 including fluid dynamics, heat and mass transfer and adsorption kinetics, seeking to identify the limiting phenomena for the rate of adsorption.

Methodology: The theory of two regions in fluidization (Cui, Mostoufi & Chaouki, 2000), in which the fluidized bed is composed of bubbles absent of solids and emulsion at minimum fluidization, has been applied, here called as the bubble-emulsion (B-E) model. In this work, the emulsion region is divided into solids and
emulsion gas, thus assuming three interacting compartments (or phases): bubble gas, emulsion gas and solids, which interact with each other through heat and mass transfer processes.
In order to describe the fluidized bed behaviour via a simplified model, the emulsion gas and solids are considered as individual perfect mixtures in the B-E model, whereas the bubble gas is represented by plug flow. The fluidized bed adsorption process is described by mass and energy balances for each compartment, correlations for distribution and behaviour of gas bubbles, bed pressure drop, heat and mass transfer between compartments and thermodynamic and kinetic models for adsorption, considering the following simplifying hypotheses:

1. System operates in steady state;
2. Emulsion gas and solids are separately perfect mixtures;
3. Bubble gas is in plug flow;
4. Emulsion region remains at minimum fluidization conditions;
5. The volume occupied by solids in the bubble region is negligible;
6. Pressure is uniform along the bed;
7. Ideal behaviour of gas mixture;
8. Adsorption mass transfer is described by a Linear Driving Force (LDF) model; 9. Adsorbed gas enthalpy change is neglected in comparison to the heat of adsorption; 10. Radiant heat transfer in the system is negligible;
11. Frictional heat generation and gravitational potential energy and kinetic energy changes are

negligible;
12. Heat exchanger wall interacts only with the emulsion gas and the bubble gas.

The adsorption thermodynamics of CO2-N2 mixtures on zeolite 13XBF adsorbent particles is described by the extended Tóth isotherm model fit to experimental data. Simulations of the B-E model for adiabatic and isothermal adsorption stages have been performed, although not yet considering the heat transfer resistances between a heat exchanger and the bed. In addition, a parametric mass transfer study under isothermal conditions was carried out to analyse the system sensitivity to the mass transfer coefficients (bubble gas to emulsion gas and LDF adsorption kineics).

Preliminary results: Simulation results of the B-E model and the Equilibrium model developed by Beleli et al. (2023), which considers adsorption as instantaneous and the entire fluidized bed as perfectly mixed (absent of temperature and concentration gradients), are compared under equal conditions for adiabatic CO2 adsorption in a single-stage fluidized bed using fixed feed gas flow (G) and varying solids flow (S).
The CO2 molar fraction in the outlet gas tends to zero as S/G feed ratio increases for the Equilibrium model, whereas it decreases to a baseline level for the B-E model, maintained all other system conditions. Considering the mass transfer parametric study results, this baseline value is determined by the mass transfer resistance between bubble gas and emulsion gas. By assuming instantaneous adsorption in the B-E model, the corresponding CO2 adsorbed amount curve overlaps the full model curve at low S/G, but they depart from each other for increasing S/G feed ratios.
In the B-E model, the heat released by adsorption phase promotes heating of the solid, which then heats the emulsion gas and, consequently, the bubble gas. The B-E model predicted a temperature difference of less than 1 K between the outlet gas and solids, indicating that heat transfer is not the limiting factor in the process.
Considering the results obtained so far, one concludes that higher CO2 recoveries require higher S/G feed ratios. In these conditions, adsorption kinetics and bubble-emulsion mass transfer resistances retard the process, so that stage efficiency and CO2 selectivity become increasingly lower.

Preliminary conclusions: A simplified phenomenological and semi-empirical model to fluidized bed adsorption has been proposed. It has been found through simulations that both bubble-emulsion mass transfer and adsorption kinetics retard the process, but for sufficiently long residence times adsorption may be regarded as instantaneous. Also, simulations predict that heat transfer is not a limiting phenomenon in the process. Stage CO2 adsorption efficiencies are predicted to be in the range of 64 to 82%, indicating that process optimization using equilibrium models might be feasible to some level. The conditions of high CO2 recovery coincide with those of low stage efficiency and CO2 selectivity, suggesting the need for further investigating the operational space.

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Abstract Title: Experimental investigations of Brazilian oxygen carriers for the chemical looping combustion technology: from micro- to macroscale

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Abstract: Amongst the suite of carbon capture and storage (CCS) technologies, chemical looping combustion (CLC) stands out as a promising avenue for enhancing CO2 capture within the currently employed energy generation systems. CLC capitalizes on the utilization of metallic and/or metal oxide particles, which exhibit the capacity to engage in reversible redox reactions that enable the oxygen transfer process between distinct reactors housing air and fuel streams. The primary objective of the present study is to delve into the reactivity of the mineral ilmenite when employed as an oxygen carrier, particularly in the context of its interaction with methane as the fuel source, at the microscale. This microscale investigation serves to elucidate the fundamental phenomena underlying the process. Additionally, a quasi-one-dimensional fixed-bed reactor is tested in order to hereafter enable the assessment of the feasibility of the CLC system at a macroscale. Such an endeavour holds significance as it contributes to the advancement of Brazilian CCS technology.

Keywords: chemical looping combustion; CO2 capture; ilmenite; oxygen carriers; quasi-one-dimensional.

Introduction and Objectives: Carbon capture and storage (CCS) technologies are gaining increasing prominence in response to the pressing imperative posed by the global climate crisis. Among these, chemical looping combustion (CLC) stands out as a method that effectively decouples the combustion reactions of fuel and air by segregating them within separate reactors. This approach holds the capacity to attenuate the formation of other deleterious pollutants, such as NOx, while concurrently obviating the energy penalty associated with the intricate gas separation process necessary for the procurement of pure CO2. In CLC process, chemical species, typically comprising metal or metal oxide particles, assumes the pivotal role of an oxygen carrier (OC). The OC enables the oxygen transfer process, whereby it oxidizes the fuel and subsequently undergoes regeneration in air, culminating in a cyclic operation that iterates continuously. Ilmenite, a mineral primarily composed of iron titanate, denoted by the chemical formula FeTiO3, has garnered substantial attention as a highly promising OC, primarily due to its ready availability, low cost, and reactivity. The primary objective of this research endeavour

is to contribute to the advancement of CLC technology within a Brazilian context. To this end, a comprehensive investigation is being conducted employing distinct ilmenite ores, with a focus on discerning their reactivity and structural alterations throughout redox cycles. Currently, investigations are undertaken employing methane as the fuel at the microscale, utilizing a commercial thermobalance; and in the near future, they will be conducted within a quasi-one dimensional (QOD) fixed bed reactor.

Methodology: The ilmenite sample underwent calcination at a temperature of 1020 °C for 2h and was characterized using X-ray diffractometry (XRD), X-ray fluorescence (XRF), and Laser Diffraction particle size analysis. Essays in the thermobalance coupled to a mass spectrometer (TG-MS) were performed in a temperature range from room temperature to 950 °C, using methane diluted by nitrogen at different concentrations. The reactor was constructed with stainless steel (AISI 310), featuring an internal diameter of 32 mm. It is segmented into three distinct sections, with the central region housing the oxygen carriers, while the two ends filled with an inert alumina-based material. The reactor's design incorporates gas supply and exhaust lines situated at its termini, which are regulated by various control devices. The inlet section provides access to a pressure transmitter, while the exhaust system is directly connected to a unit consisting of a heat exchanger and a condensate collector. Three heating coils are strategically positioned along the length of the reactor to facilitate precise temperature control during the initial phases of operation. The entire process, encompassing control and data acquisition, will be executed with the assistance of 27 thermocouples affixed to the reactor, and the gases generated during the process will be analysed via an integrated infrared gas analyser.

Preliminary results: Experimental findings reveal that calcinated ilmenite primarily consists of the pseudobrookite phase (Fe_2TiO_5), hematite (Fe_2O_3), and rutile (TiO_2), with a minor presence of quartz (SiO_2), exhibiting a particle size of approximately 70 µm. TG/DTG-MS curves demonstrate that the active phases involved in the reduction of calcinated ilmenite under a 25% methane atmosphere commence at temperatures of approximately 700°C, marked by the detection of CO_2 and water mass fragments. No discernible reactions were observed for lower methane concentrations. Regarding the fixed bed reactor, the quasi-one-dimensional (QOD) system is currently undergoing preliminary tests. At this juncture, emphasis is being placed on evaluating the system's airtightness at elevated temperatures, thereby gauging the efficiency of the heat exchanger. Further operational tests are being conducted with the objective of refining the control and data acquisition devices, as well as optimizing the operational programming of the Programmable Logic Controller (PLC).

Preliminary conclusions: The selected ilmenite sample, employed in reactivity tests involving methane, has demonstrated effective fuel oxidation at elevated concentrations. Nonetheless, it is imperative to investigate a range of parameters, including various fuel concentrations, to acquire comprehensive insights essential for guiding subsequent quasi-one-dimensional (QOD) reactor operations. Simultaneously, the progression of the reactor's development, from its initial

design phase to achieving operational conditions, is furnishing us with the requisite knowledge necessary for the forthcoming operational commencement. This, in turn, will unlock prospects for the inception of novel projects within the chemical looping combustion (CLC) domain.

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Abstract Title: Labyrinth Diode Designed by Topology Optimization of Binary Structures using Laminar Flow and Real Gas Properties with Experimental Validation

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Abstract: One of the most pressing issues that require attention is the reduction of CO2 emissions, and one approach to mitigate this problem is by enhancing the performance of diodes used for sealing and minimizing leakage in turbomachinery. This study focuses on the design of a labyrinth diode using the Topology Optimization of Binary Structures (TOBS) method, which incorporates laminar flow and real gas properties. The labyrinth diode design is obtained through TOBS, considering energy dissipation and vorticity magnitude as a multi-objective framework within a specified volume fraction. The optimization problem takes into account the dimensions of the test bench and the properties of real CO2 gas in a two-dimensional axisymmetric model. The labyrinth diode design is optimized for laminar fluid flow governed by the Navier-Stokes equations, with the inclusion of the standard Darcy term to penalize solid domain infiltration. Computational Fluid Dynamics (CFD) is employed to numerically assess the diode's performance and compare it with experimental measurements, evaluating its effectiveness in reducing leakage. The optimized topology is transformed into a solid model and fabricated using UV-photosensitive resin through 3D printing. The fabricated prototype is then tested on a test bench (TB) equipped with a chamber capable of evaluating two seals with a middle entry, utilizing a 40 mm rotor. The TB can reach a maximum rotational speed of 10,000 rpm and generate a pressure drop of up to 5 bar. The leakage rate is measured in kg/s using instrumentation that adjusts the mass flow rate based on pressure/temperature analysis. The results indicate the need for further improvements to accommodate turbulent flow and higher Mach numbers in compressible flow during Topology Optimization. Nonetheless, the findings offer promising
insights into reducing leakage in turbomachinery seals.

Keywords: Topology Optimization, Labyrinth Diode, Laminar Flow, Experimental Validation.

Introduction and Objectives: Earth's temperature is regulated by the greenhouse effect and naturally occurring atmospheric greenhouse gases [1]). Post-Industrial Revolution, human

activities escalated CO2, CH4, N2O, and F-gas emissions, intensifying warming [2]. Resulting in climate change challenges global governance [3]. Scientists stress emission reduction [2], evident in treaties like Kyoto Protocol and Paris Agreement. Notably, methane (CH4) with an energy absorption capacity 84 to 87 times greater than CO2, is a key contributor; in the US, 40% of 2019 emissions were from energy, 60% from natural gas systems [4], partially due to machinery leaks. Labyrinth seals help counter leakage, preserving fluid control. The labyrinth seals constitute a type of non-contact annular seal. They typically employ flow restrictions and cavities with the purpose of minimizing leakage or escape flow [5, 6]. The seal delineates a high pressure region from a low-pressure one, and these regions can exist either between two stages of fluid machinery or between the internal and external regions of turbomachinery [7, 8]. When compared to other types of annular mechanical seals, labyrinth joints prevent friction between components, thereby contributing to an enhancement in the performance of fluid machinery [9]. Additionally, owing to their low cost, simple assembly, and high reliability, labyrinth seals constitute the majority of mechanical seals employed in turbomachinery [10–12], such as compressors, turbines, and turbochargers. There are a few test benches for experimental validation of Labyrinth Seals. It's possible to list some as the Turbomachinery Laboratory at Texas A&M University or the Southeast University setup in China which measures the vibration effect duo different geometries labyrinth seals. Booth Test Benches are helpful, but in this paper, we're interested only in leakage, pressure, and rotation conditions. Fluid flow Topology Optimization (TO) was introduced by Borrvall and Petersson [15] pursuing the path with minimum energy dissipation assuming a Stokes flow using continuous variables (or pseudo-densities approach). This paper aims to demonstrate a generic framework for manufacturing and testing prototype designs of topology-optimized labyrinth seals. The efficient generic mathematical programming of the TOBS method has shown potential for topology optimization computations for fluid flow applications (laminar regime [18], rotating flow [23], turbulent models [21] and subsonic compressibility effects [24]) using integer design variables. Therefore, we chose this binary approach in order to obtain novel designs that reduce leakage in turbomachinery. Finally, the reliability of the design is verified, the prototype is manufactured using 3D printing and tested in a TB. The flow rate is compared at the same pressure and rotation conditions.

Methodology: Fluid Flow Governing Equations for Topology Optimization.

The fluid particle motion in a fluid domain **Ω** is modeled in the laminar regime assuming: i) constant density ρ and dynamic viscosity μ; ii) absolute velocity v and the pressure p fields independent of time; and iii) negligible body forces. Thus, the steady incompressible Navier-Stokes flow equations can be expressed as [25]:

$$\rho\,(v \cdot \nabla v) = -\nabla p + \mu \nabla 2v, \quad (1)$$

$$\nabla \cdot v = 0. \quad (2)$$

where Eq. 1 is the conservation of momentum and Eq. 2 is the continuity equations.Usually, fluid problem definitions include: the fluid entrance as the inlet (Γin); the exit as an outlet

(Γout); and the solid frontier in inner flows as the fluid walls (Γwall). Herein, a fully developed inlet velocity profile, zero stress outlet, and no-slip conditions on fluid walls are adopted. The prescribed boundary conditions assumed are:

v = vin on Γin, (3)

−pI + ∇v · n = 0 on Γout, (4)

v = 0 on Γwall, (5)

Classic fluid TO literature emulates solid regions as porous material with low permeability [15]. Therefore, a material model expression (Darcy term) must be added to the governing equation to emulate the regions in which the fluid is removed with resistance forces proportional to the velocity. This implies that only non-zeros design variables will have interpolated properties equal to the assumed maximum inverse permeability value κmax. Thus, the laminar flow governing equation (Eq. 1) is rewritten as the generalized Navier-Stokes equations including the Darcy friction term: ρ (v · ∇v) = −∇p + μ∇2v − κ(x)v.

Topology Optimization Problem:

In order to solve the seal problem, boundary conditions were imposed on forward and backward flow directions. In these devices, the geometry can be designed to favor the flow in the desired direction while increasing the resistance on the opposite direction, similar to a Tesla valve [26]. However, the traditional expression used to maximize diodicity is susceptible to an undesired local minimum which closes the channel (creates a solid region
that obstructs the flow path). Therefore we achieve the diodicity maximization by combining energy dissipation and vorticity on opposed flow directions (instead of the classical approach that uses only energy dissipation terms). The fluid viscous energy dissipation E(x) and the vorticity Φ(x) in the 2D axisymmetric space can be expressed related to the radial coordinate r as:

$$E(x) = \int_{\Omega} \left(\mu 2 \, \|\nabla v + \nabla v^T\|2 + \kappa(x)\|v\|2 \right) 2\pi r \, d\Omega,$$

$$\Phi(x) = \int_{\Omega} \|\nabla \times v\| \, 2\pi r \, d\Omega.$$

In this paper, we perform diodicity maximization by minimizing the forward energy dissipation Ef orw while maximizing the backward vorticity Φback subjected to a fluid volume constraint V (x). Therefore, the topology optimization problem is given by:

Minimize

x F = w1 · log (Ef orw(x)) − w2 · log (Φback(x))

https://docs.google.com/forms/d/1bkctUbioK8sVvBHdbBjZ6cTw26p0wlPbgrru1pI3Jbg/edit#

Subject to V (x) ≤ V ,
xj ∈ [0, 1]

where V is the prescribed volume fraction, and w1 and w2 are weight parameters used to control the dominance of effects. We ensure the proportion w1 + w2 = 1.

Preliminary results: Figure 4 presents the topology obtained after the optimization procedure and the solution of the velocity field at the direction that was designed to impose higher resistance to the flow. In order to show only the flow at the designed fluid path, we performed post-processing of the topology boundaries to smooth the staircase contour. Observe that the seal design favored the emergence of two recirculating regions.
These interlaced vortices chambers
contribute to making a long path to dissipate more energy on the seal mechanism. After getting this result, a full geometry for the test bench has been done, coupling two TO results in series. With that geometry, a simulation was made using ANSYS Fluent®, with compressible and turbulent flow, using (a) Optimized topology for seal design chamber (b) Velocity field on backward flow

Figure 4. Solution of the topology optimization of the seal problem.

K- ωSST turbulence model, in a 2D-axisymmetric swirl flow domain, stationary (Pseudo-Transient), with real gas properties (Soave-Redlich-Kwong air model). The Pressure and Velocity results are shown in Fig. 5.

(a) Pressure Field
(b) Velocity Field
Figure 5. Compressible Turbulent Flow CFD results

Prototype Manufacturing for Experimental Validation

The first step is to convert the TO result into a CAD file. For this task, it's used the software SOLIDWORKS® to create a sketch extracted from the design domain and then revolutionize it, generating volumetric bodies. The stator was divided into two parts with pins for guided assembly. Utilizing Halot Box® software, the printable file was obtained and used to produce the prototype on a Creality Halot Sky 3D printer. This printer uses UV-cured
grey resin with a 4K resolution 9.25" screen, ensuring high-quality layering at 0.05 mm height.

Post printing, parts underwent a 10-minute external cure in two different orientations. The labyrinth diode prototype's manufacturing steps and final assembly are illustrated in Fig. 6.

(a) 3D Printing process
(b) UV external cure
(c) Labyrinth Seal Assembly
Figure 6. Manufacture Process

The printed Labyrinth Seals are tested in our Test Bench at USP. The Test Bench is equipped with a chamber capable of evaluating two seals with a middle entry, utilizing a 40 mm rotor.

The setup can reach a maximum rotational speed of 10,000 rpm and generate a pressure drop of up to 5 bar. The leakage rate is measured in kg/s using instrumentation that adjusts the mass flow rate based on pressure/temperature analysis, also shown in Fig 7.

(a) Test Bench Overview (b) Measure Instrumentation
Figure 7. Labyrinth Seal Test Bench at USP

The distance between the results is evident, yet it remains a calibration and testing time issue. Moreover, tests will be conducted using the TO Labyrinth Seal to compare leakage and validate the effectiveness of the TO methodology.

Figure 8. Experimental Results and CFD

Preliminary conclusions: This paper proposed a general framework for manufacturing prototypes with optimized designs is proposed by using additive manufacturing equipment. The Topology optimized design was obtained considering a simplified flow condition in the two-dimensional axisymmetric model assuming laminar incompressible CO2 in realistic test bench dimensions. The CFD is used to guide experimental validation but is still under parameters calibration to get closer to the experimental. The proposed framework to manufacture the Labyrinth Seal using addictive manufacture has proven efficient. The Measuring process looks nice and efficient, but still a work in progress, under calibration. The proposed analysis serves as a recommendation for future works on verifying and prototyping optimized labyrinth fluid diodes. Topology Optimization for test bench pressure conditions and experimental comparison of performance with baseline seals are future directions of this research.

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Abstract Title: Solid Oxide Fuel Cell (SOFC) channel design using the Topology Optimization Method

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Abstract: Energy sources are mostly dependent on fossil fuels, which have negative environmental effects. As a result, the use of alternative energy sources is becoming even more crucial. In this context, internal combustion engines and other conventional energy conversion technologies are being replaced by fuel cells. Fuel cells generate energy by electrochemical reactions, which makes it considerably cleaner and more sustainable than traditional combustion-based technology. In this context, the design of fuel cells based on the topology optimization method is a powerful approach to finding alternative and non-intuitive design configurations for both gas and air channels. For that, a cell-level model is considered to incorporate processes on the macro-scale as gaseous species transport and on the micro-scale as gaseous diffusion, electrical/ionic conduction, and electrochemical reactions. Here, effective transport or reaction parameters are used to consider the micro-scale processes on the cell level. The topology optimization problem is formulated aiming to design fuel and air channels in an SOFC fed by hydrogen in a way that the efficiency in energy generation is maximized.

Keywords: Topology Optimization, Solid Oxide Fuel Cells, Multiphysics Simulation.

Introduction and Objectives: There is a growing demand for energy sources that currently are mainly dependent on fossil fuels, which are limited resources and have severe environmental impacts. Consequently, energy diversification and the employment of alternative energy sources are becoming even more important. In this context, fuel cells are a leading alternative to conventional energy conversion devices, such as internal combustion engines. The energy generated by fuel cells comes from electrochemical reactions: the chemical energy of the organic load of the biomass resources is converted directly into electricity, which makes it much cleaner and more sustainable than conventional combustion-based technology. The main objective of this research is the development of advanced methods for Topology Optimization of SOFC at cell channel designs with improved performance.

Methodology: Initially, the proper formulation to describe the electric, ionic, and gaseous species transport in the porous media is derived. Real properties and suitable empirical relations to model the electrochemical charge transfer reactions are selected based on the literature. Then, the numerical model is implemented using the finite element method to describe the SOFC cell layer behavior in terms of velocities, pressure, mass fractions for the species in both fuel and air channels, and local current densities. Thus, the optimization problem is defined aiming at

improving the cell power, and the design algorithm is implemented based on topology optimization to deal with the multiphysics simulation by employing suitable material models.

Preliminary results: Preliminary results were obtained for the topology of the SOFC fuel and air channels, so that the cell power is maximized. The optimized solutions are compared with generic configurations, such as serpentine, to evaluate the proposed optimization methodology.

Preliminary conclusions: The Preliminary results demonstrate the ability to obtain non-intuitive solutions through the topology optimization method, which can result in cell designs with improved energy efficiency.

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Abstract Title: Digital Transformation Process Based on Automation and Data Service: a case study in sustainability projects

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Abstract: The process of digital transformation propagates throughout the domain of (automated) services and opens up the possibility for cloud services to tend to ubiquitously permeate all human activities, from primary (agricultural) production to assistance and leisure services, passing through for industrial production, fulfilment services and even startups. The diversity of applications creates a even greater demand for theoretical development in service system design methods as well as in the adaptation of these models to the respective domains of application. With respect to design methods the objective is to propose a project cycle (forthe digital transformation strategy) in Model-Based Systems Engineering (MBSE) capable of flexibly capturing the demands of users and stakeholders, and trigger the adaptation phaseto the application domain with a formal framework. A case study will be the basis for experimentation, linked to the modelling of greenhouse gas emissions in the Amazonian rainforest, a good challenge in terms of complexity and innovation. The design cycle includes the use of requirements analysis techniques, "data lake" treatment, the use (and reuse) of already known processes and of Intelligent Planning (IA Planning).

Keywords: Digital Transformation, Services Engineering, MBSE, Amazonian rainforest, Data Lake.

Introduction and Objectives: Forest monitoring implies measuring and recording a set of forest variables in a time 14 series that become available to track its changes. Monitoring forests is necessary for 15 preserving sustainability policies and climate change contexts since forests are essential 16 carbon stocks. For example, in Brazil, approximately 46% of all CO2 emissions primarily 17 originated from forests and land manipulation, as shown in a for 2020.
This work focuses on developing cloud data services to support analysis and reduce maintenance costs, which might also reduce implementation costs and time. In the science domain, those are desirable advantages that can improve analysis capacity and enhance the capacity to compose historical data, a necessary feature in asynchronous Forest Digital Twin, which uses cloud computing technology based on Data Lake to propose a reference framework for services in the Amazon Web Services (AWS) cloud aimed at manipulating data transmitted over the web. The proof of concepts will be this data lake used to provide basic services to search for appropriate datasets for modelling greenhouse gas emissions coupled with the "Greenhouse gas emissions in the Amazon and data analysis system and services" (RCGI GHG D1.1 project) with the objective of reducing greenhouse gas emissions in the Amazon. This work addresses two contributions: the first is a bibliometric review of cloud data repositories connected to digital transformation; the second is a proposal for the early design of cloud service for cutting-edge systems applied to research in sustainability.

Methodology: The scientific data sharing system is designed to facilitate the exchange
efficient and secure exchange of metadata and files between researchers and scientists. This system will be hosted in the AWS cloud, taking advantage of its scalability, robustness and resources advanced security features.

The system will be able to integrate and synchronize with an existing on-premise system. This synchronization capability will allow for a seamless workflow between the cloud environment and the on-premise environment, ensuring that all metadata and files are consistently up to date on both platforms.

Furthermore, the system will include a web interface through which users can perform queries to search for metadata and files. This web interface will provide an intuitive, easy-to-use way for users to access and explore data stored in the system.
The implementation of the system will also involve the creation of a datalake to store and organize metadata and shared files. The datalake will be designed to enable efficient queries and will offer a high level of flexibility in terms of types of data that can be stored.
The scope of this system focuses on the implementation and management of these functionalities and capabilities. The system will not include the development of new analysis algorithms of data or carrying out scientific research using the shared data. In addition, Furthermore, the system is not intended to completely replace any IT infrastructure
existing on-premise system, but rather to complement it and expand its capabilities.
The scientific data sharing system is being developed as part of the GHG D1.1 project (Greenhouse Gas Emissions in Amazon and Data Analytics and Service System). The main objective of this project is to study gas emissions greenhouse effect (GHG) in the Amazon

Forest and provide analytical tools for researchers and scientists in this field.
This system is designed to serve as a robust and reliable, providing functionalities that add value to the processes necessary to analyse GHG data from the Amazon Forest. Among these features are data acquisition, secure data storage, synchronization with systems
on-premise and the ability to execute complex queries and visualizations of data. Automation plays a significant role in product vision, with many of analysis processes being automated to increase efficiency and reduce probability of errors. However, the first version of the system will be focused on creating of services that facilitate the acquisition of data from sensors and data collection equipment data, as well as existing databases and files and visualization using a web information system in the cloud.

Preliminary results: The platform is cloud-based, structured on AWS. The system is composed by several components that work together to extract, transform and load data from different sources into a centralized datalake.

The datalake receives metadata and scientific data sets from various sources, including relational and non-relational databases, a web information system and an on-premise system. Synchronization of new and modified system files on-premise is managed by a local mini Kubernetes cluster, which runs Apache Airflow with DAGs (Directed acyclic graph) specific for this purpose. Authentication for the information system is managed by the AWS Cognito service.
Furthermore, a replica of the web information system is maintained in the on-premise system, allowing local researchers to contribute datasets that are later synchronized to the cloud via Rest APIs.
In the cloud, a Kubernetes cluster is used to manage the instances of a
Kafka Enterprise Service Bus and Apache Airflow. Data is sent and received from the Kafka bus, which also integrates with Rest APIs.
The on-premise system sends metadata and files through the Rest and AWS Client APIs Services, which deliver data to Kafka for processing. Local Airflow syncs
new and modified data with the on-premise system, and distributes the data across databases Datalake and Information System dataset.
Users can consult, download and analyse scientific data using the cloud-based information system. User queries are managed by AWS Elastic Search service, with plans to incorporate a Machine Learning trained from a graph database to improve effectiveness and relevance of research.
Partners can integrate directly with the cloud information system through Rest APIs, providing an efficient means of collaboration and data sharing. The administration of AWS services is accessed via SSO - Single Sign On, which allows you to create and configure new services as necessary for the operation of integration between cloud and on-premise systems.
We use Petri Nets, a powerful tool for modelling and analysing systems that deal with competition, synchronization and shared resources. Through the simulation of our approach

tosynchronization in the Petri Net, we were able to identify and prevent deadlock situations that could potentially occur during the synchronization process. Once satisfied with the performance and security of the synchronization process in the simulation, we implement the solution in the real system.
Data synchronization between the cloud system and the on-premise system is managed through a set of highly coordinated processes, which includes the use of DAGs (Directed Acyclic Graphs) distributed by Apache Airflow, the service bus
Kafka, Api's Rest and several S3 buckets.

Preliminary conclusions: The system features an advanced and integrated digital infrastructure, designed for management, research and dissemination of scientific data, especially in the context of studies related to gas emissions in the Amazon Forest. With a variety of functionalities such as dataset management, user profile, of news and curation, it provides a robust platform for researchers, collaborators and the general public.
At the core of the system, the data set management module allows researchers to upload, update and manage crucial information in formats NetCDF, HDF and GRIB, thus ensuring data integrity and accessibility. An integration between microservices, using technologies such as Kafka and Apache Airflow in a Kubernetes environment, highlights the modern architecture of the system, allowing for a fluid and scalable operation.
The focus on accessibility and usability ensures that the user interface is intuitive, promoting an enjoyable experience for all users, regardless of of their technological familiarity. Furthermore, strict security policies, which include encryption and data protection, ensuring confidentiality and integrity of information, even in a scenario where much of the data is publicly accessible.
Therefore, this system serves as a framework for scientific research platforms, combining advanced functionalities with security and ease of use. It not only facilitates research and collaboration between experts, but also establishes itself as a reliable source of information for the general public, thus strengthening knowledge sharing and collaboration in the field of environmental science.

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Abstract Title: Use of Automated Low-Cost Sensors for Methane (Ch4) Emissions Monitoring

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Abstract: It is proposed to test the behavior of low-cost commercial sensors from Figaro Engineering Inc., methane (CH_4), and carbon dioxide (CO_2) gas meters, integrated into printed circuit boards. The study method consists of comparing measurements obtained by the low-cost sensors connected to a logger and by more robust methods or equipment available on the market (ABB Group Greenhouse Gas Analyzer). In the absence of a greenhouse gas analyzer installed at the target monitoring site, gas samples are collected for later analysis in a gas chromatograph (GC). After data acquisition, a comparative analysis is conducted to assess and understand the operation of the sensors in the specific context. So far, two large datasets have been obtained. The first one contains emission data resulting from a

controlled methane (CH_4) leakage experiment, in which, alongside the sensors, the portable gas analyser from the ABB Group previously mentioned was used. As for the second dataset, it was collected during the first phase of the Trans-Amazon Drilling Project (TADP), in a drilling operation in the sedimentary basin of Acre, in Rodrigues Alves, Acre. In this operation, sensor boards were installed at the gas outlet from the well, alongside two gas chromatographs (GCs). Up to this point, it has been concluded that variables such as air humidity, oxygen (O_2) gas concentration, amperage, and voltage of the power source interfere with the sensor's operation. They have a high capacity to determine variations in greenhouse gas concentrations over extended periods of time. Improved methodologies should be applied to ensure their proper field operation, and calibration methods should be established for future, more robust analyses.

Keywords: Methane, CH4, Sensors, Greenhouse gas, GHG, Greenhouse gas analysers.

Introduction and Objectives: It is proposed to test the behaviour of low-cost commercial sensors from Figaro Engineering Inc., methane (CH4) and carbon dioxide (CO2) gas meters, integrated into printed circuit boards developed by Bastviken et al. (2020). From this, the aim is to study the functioning of this experimental system when applied in real situations, contributing to the expansion of access and the spatial and temporal resolution of greenhouse gas (GHG) emission data acquisition in projects and ventures in Brazil.

Methodology: The study method consists of comparing measurements obtained by low-cost sensors connected to a logger with those obtained by more robust methods or equipment available on the market (Greenhouse Gas Analyzer). In the absence of a greenhouse gas analyser installed at the target monitoring site, gas samples are collected for subsequent analysis in a gas chromatograph (GC).
Following data acquisition, a comparative analysis is conducted to evaluate and understand the

functioning of the sensors in the specific context. In addition, continuous literature review is carried out on greenhouse gas emissions and gaseous hydrocarbons to the atmosphere, as well as on the operation of the gas meters in question, which are of the metal-oxide-semiconductor (MOS) type.

Preliminary results: So far, two large datasets have been obtained. The first dataset contains emission data resulting from a controlled methane (CH4) leakage experiment conducted in collaboration with researchers from the Centre for Lasers and Applications (CLA) at IPEN - USP. In this experiment, alongside the sensors, a portable gas analyser from the ABB Group, widely used in the market, was employed. As for the second dataset, it was collected during the initial phase of the Trans-Amazon Drilling Project (TADP) at a drilling site in the sedimentary basin of Acre, in Rodrigues Alves, Acre. Sensor boards were installed at the gas outlet from the well, along with two gas chromatographs (GCs) responsible for monitoring the gases discharged with the drilling fluid used to maintain well stability. In the CLA experiment, the controlled leakage involved an Ar-CH4 (10%) gas mixture and lasted approximately 1 hour and 30 minutes. The values recorded by the ABB analyser ranged from 2000 to 3000 parts per million (ppm), while the sensors under study reached their maximum reading value at 2047 millivolts (mV). In the TADP test, while the GCs measured CH4 levels at 80 to 120 ppm, the sensors recorded readings in the range of 1100 to 1200 mV.

Preliminary conclusions: Variables such as air humidity, oxygen gas (O_2) concentration, amperage, and voltage of the power source interfere with the sensor's operation. They possess a high capacity to detect variations in greenhouse gas concentrations over extended periods of time. Improved methodologies should be applied to ensure their proper field operation by analysing the conditions under which the sensors will be subjected in relation to the mentioned variables. Additionally, calibration methods should be established for future, more robust analyses.

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Abstract Title: Topology optimization of Turbulent 2D swirl Fluid-Structure Interaction Problems Applied to Labyrinth Seals Design Considering Natural Frequency Constraints

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Abstract: This work is associated with the project " Design of smart labyrinth seals for mitigation of GHG emissions in pneumatic machines". Labyrinth seals are a type of mechanical seal located between the stator and rotor. These devices operate with tight assembly tolerances, leading to wear problems caused by excessive vibrations. In this context, it's crucial to enhance the design of these components to reduce vibration levels and avoid resonant conditions. This study focuses on topology optimization for turbulent 2D swirl fluid-structure problems while considering natural frequency constraints. The governing equations are solved using separate domains and the k-w turbulence model with standard wall functions. The optimization method employed is TOBS-GT, which separates the Finite Element Analysis (FEA) module (COMSOL Multiphysics) from the optimization module, facilitating sensitivity interpolation between the meshes of these modules. Compliance sensitivities are computed through automatic differentiation using a built-in optimization module in COMSOL Multiphysics, while natural frequency sensitivities are derived analytically and implemented in MATLAB. Numerical results explore the optimization of 2D axisymmetric labyrinth seal geometries, encompassing the design of teeth and the stator while adhering to predefined natural frequency constraints. The results underscore the potency of topology optimization as a valuable tool for devising innovative labyrinth seal structures with natural frequency considerations.

Keywords: Topology optimization; Integer Linear Programming; Non-linear constraint; Turbulent flow; Labyrinth seals.

Introduction and Objectives: Topology optimization (TO) is recognized as a modern computational tool that generates highly innovative designs in structural systems, but its application is somewhat limited when it comes to multiphysics problems such as Fluid-Structure Interaction (FSI). In engineering applications, FSI modelling plays a vital role in the design of various systems, including turbomachinery, airfoils, engines, and offshore structures like subsea risers and wind turbines. In some cases, simplifying the loads acting on a structure is sufficient to produce efficient designs. However, there are situations where the physics involved in the structure results in complex and design-dependent loads that cannot be easily simplified or ignored. Take, for example, labyrinth seals in turbomachinery, which are critical components of modern aero-engines and are susceptible to wear and failure. Interference between the seal rotor and stator often occurs, leading to damages such as break-offs, bending, mushrooming, or rub grooves. These damages alter the clearance from the original design, significantly impacting the labyrinth seal's real-world performance compared to its initial design. A labyrinth seal is a specific type of mechanical seal located between the stator and rotor in these mechanisms. Fluid repeatedly passes through the gaps, generating kinetic energy that dissipates in the downstream inter-fin cavity. This process results in pressure losses that

reduce leakage flow through the seal. Experimental observations have indicated that labyrinth seals are susceptible to flutter, a phenomenon where acoustic waves in the interfin cavities match the natural frequencies of the seal, potentially causing instabilities, wear, and equipment failure due to rotor-stator interference. However, tackling seal flutter is a complex issue that is currently not feasible with topology optimization. Consequently, our research aims to progress incrementally throughout the Ph.D. research. Accordingly, this study proposes designing labyrinth seals through topology optimization while considering them as FSI problems. This involves accounting for turbulent fluid flow and managing the structure's natural frequency to control vibration levels.

Several strategies have been employed to address topology optimization for design-dependent FSI loads. Recently, an innovative technique using binary design variables has been developed, which incorporates an explicit boundary method with the Topology Optimization of Binary Structures (TOBS) method by merging numerical tools and methodologies to integrate them. Notably, in the realm of TO FSI literature, to the best of the author's knowledge, there are no works that consider turbulent fluid flow or natural frequency constraints. In light of this, this research stands as innovative in its integration of turbulent flow and nonlinear constraints (natural frequency) using sequential integer linear programming for labyrinth seal design.

Methodology: The optimization is performed using the Topology Optimization of Binary Structures with Geometry Trimming (TOBS-GT) method, which separates the optimization and FEA meshes using binary design variables. The optimization is carried out in MATLAB via the TOBS implementation. The forward FSI problem is solved with COMSOL Multiphysics. The compliance sensitivities are calculated in COMSOL Multiphysics via semi-automatic differentiation and the natural frequency sensitivities are obtained via analytical expression. To ensure that the frequency of interest is properly restricted, the modal assurance criterion-based (MAC-based) mode-tracking method is used to identify mode crossing during the optimization process.

In summary, the main steps of the algorithm employing the TOBS-GT method are as follows:

1. Define the optimization parameters.
2. Create the optimization grid and assign an initial {0, 1} topology.
3. Extract the geometry from the optimizer mesh and smooth it.
4. Generate a CAD file as a .dxf file for a 2D analysis.
5. Export the CAD file to COMSOL Multiphysics® where the forward problem and adjoint sensitivities are calculated.
6. Filter the sensitivities of the problem (natural frequency and compliance) to be added to the optimizer.
7. Update the design variables using the ILP solver.
8. If converged, stop. If not, iterate from step 3.

Preliminary results: Three numerical examples are explored to study the design of the labyrinth through topology optimization, considering a Fluid-Structure Interaction (FSI)

problem. These examples include: a seal with one tooth, a seal with two teeth, and the stator structure.

In the case of the seal with one tooth, the tooth on the rotor is subjected to three rotational speeds: 0 rpm, 1000 rpm, and 2000 rpm, with a Reynolds number of 10,000. A natural frequency constraint of 65,000 Hz is used. In this example, we can observe the equilibrium between the loads caused by the rotational body force and the FSI loading. It becomes apparent that as the rotational body force increases, the optimization becomes less stable.

For the seal with two teeth, the same three rotational speeds (0 rpm, 1000 rpm, 2000 rpm) and Reynolds number are employed. A natural frequency of 55,000 is defined. In this case, one tooth is located on the stator, and another is on the rotor. The goal is to analyse the influence of the topology evolution when one tooth is subjected to rotation and FSI loading, while the other experiences FSI loading only. It is evident that the topology of the tooth subjected to rotational speed affects the topology of the tooth subjected to FSI loading only.

In the final example, the optimization focuses on the stator structure while considering the teeth as non design domains. The objective is to maintain the fluid flow path and control the natural frequency in the stator structure. This example involves a rotational speed of 20,000 rpm applied to the rotor walls, and the stator is optimized with a natural frequency constraint set at

55,000 Hz.

Preliminary conclusions: A study of turbulent 2D swirl topology optimization of FSI problems considering natural frequency constraint applied to labyrinth seals is performed. The optimization problem of compliance minimization subjected to a volume and natural frequency constraints is solver. The results ensure that the method works to increase the natural frequency of structures subjected to a turbulent fluid flow. For teeth optimization, stiffer structure with increased natural frequency were obtained. However, the manufacturing of these structures is complex. Another point is that the wet optimization tends to worse the fluid flow optimization. So, a complementary analysis considering the stator as design domain was carried out.

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Abstract Title: Decarbonization policies in the industrial sector: a systematic revie

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Abstract: The industry plays a key role in the GHG mitigation strategy of all countries because the sector has high representativity in the share of emissions that reached 24% with 14 GtCO2 in 2019. Moreover, the sector's development is associated with the economic growth rates monitored yearly by the international market. However, this growth must be followed by the premises of sustainability and be guided by the NDCs established in the Paris Agreement. To enable this successful advance in economic efficiency linked to sustainability, it is essential to adopt different policies. This study aims to develop a literature review of public policy proposals directed to the industry and its subsectors and evaluate the success mechanisms or gaps that still need to be filled to promote the sector's progress with the established GHG

neutralization targets.

Keywords: GHG, Industrial Emissions, Policies.

Introduction and Objectives: According to the United Nations forecasts, by 2022, the global population will have reached 8 billion people. In this sense, we see the demand for products and services increasing considerably and the industrial plants of the most diverse subsectors expanding and requiring high levels of energy. The International Energy Agency reports that industrial emissions have increased by more than 70 percent since 2000 as a result of the increased demand for industrial goods. Most materials are traded in the commodity markets based on standard products, large volumes and price competition. (Åhman, et al., 2017). Therefore, the current economic models associated with the growth needs for basic materials make the industrial sector a major contributor to the GHG neutralization targets. In the last decade, the industrial sector has been trying to minimize its emissions by increasing the results of energy efficiency, use of biofuels, and production optimization. But ensuring the scalability of these solutions requires adopting new solutions for the business model, financing capacity, and a stable market environment. In response to this global ecological and societal challenge, many organizations are quickly stepping up their activities to develop and deploy more aggressive GHG reduction strategies. An essential element for institutions to successfully meet the climate change challenge will be identifying effective strategies and corresponding initiatives that lead to cost-effective reductions in GHG emissions (Meissen & Eagan, 2018). In this sense, the literature has shown that the industrial and energy sectors have changed the type of fuel, switching to less carbon-intensive fuels. However, this change will hardly reduce

emissions above 80% (Wilson & Staffell, 2018). To address the challenges posed by GHG emissions in manufacturing, collaboration between governments, industry stakeholders, and research institutions is vital. For this reason, this article evaluates existing policies focused on the manufacturing sector in order to mitigate GHGs. Public policies establish ambitious goals and targets, promoting energy efficiency and transitioning to sustainable manufacturing practices. These goals provide a clear direction and create a sense of urgency for manufacturers to invest in sustainable technologies. Therefore, this study intends to understand the mechanisms adopted by the policies and the solutions of those that have succeeded in their objective and, finally, to understand the gaps that still need to be filled.

Methodology: This paper aims to highlight potential gaps in existing policies through qualitative analysis of articles and reports that bring precise results on applying such policies in different industry subsectors. The methodology proposed consists of a Systematic Literature Review (SLR)of articles with adherence that include analyses of policies focused on the industrial sector. The Systematic Literature Review (SLR) is an academic investigation that allows the identification, selection, evaluation, and synthesis of relevant evidence available on a given research object (Galvão; Pereira, 2014). In order to obtain more detailed results, the specific research objective focuses on categorizing the articles based on the applicability of each policy by identifying the sub-sector addressed. Initially, using the PICO protocol, the main parameters of the research were defined. This structure is the most commonly used to define a reseachable question, which specifies the type of Patient or Population, type of Interventions (and Comparisons if there is any), and the type of Outcomes that are of interest (The Hong Kong Polytechnic University, 2023). In the second phase, the “Preferred Reporting Items for Systematic Reviews and Meta-Analyses” (PRISMA) protocol was used in order to critically analyze all articles and their adherence to the research scope. The use of PRISMA is primarily intended for the development of protocols for systematic reviews and meta-analyses that synthesize aggregated data from studies, particularly on evaluations of the effects of interventions (Moher et al., 2015).

Preliminary results: The literature search resulted in the selection of 25 relevant documents. The articles actually accepted at the screening phase were assessed and categorized by sector type (e.g. steel and iron, chemical, pulp and paper, etc.) and country. The results show that the articles address the problem of greenhouse gas emissions in the industry globally making comparisons between countries and highlighting which technological solutions can make the neutralization targets feasible. Looking at the sectors analyzed, it was observed that the steel industry had the largest participation in studies performed (24%), followed by the cement industry (16%), EIIs (16%), Industry in general (12%), Oil & Gas (12%), Ceramic Industry (4%), Chemical Industry (4%), Commercial systems (4%), Forest Industry (4%) and Manufacturing (4%). The 3 most frequently cited policies, or policy models, among the articles were the European Union Emissions Trading System (3 citations), Carbon Pricing (3 citations), European Green Deal (2 citations) and Paris Agreement (2 citations). It is worth noting other policy citations that also had only one citation:

• Carbon tax;

• Cross-sector emissions reduction targets and harmonization of policy frameworks; • Directive 2003/87/EC;

• Directive 2009/29/EC;

• Directive 2012/27/EU;

• Emissions intensity targets based on geography or industrial sector;

• Energy Efficiency Standards;

• G7 Industrial Decarbonisation Agenda;

• Green Industrial Policy;

• High-Level Expert Group on Energy-Intensive Industries;

• Net-Zero by 2050;

• Prioritization of novel decarbonizing interventions to "hard-to-decarbonize" sectors; • Technology Investment Roadmap for low-emissions technologies;

• The 2050 Net Zero Global Industry Roadmap of the Global Cement and Concrete. The qualitative analysis of the 25 articles elucidated the fact that from a technological point of view, there is a clear difficulty in expanding decarbonization projects such as CCUS due to the capital intensive characteristic of these projects. In general, stakeholders in the industry have a clear view of the state-of-the-art technology that researchers have presented as a solution to achieve the neutralization goals, but the scalability of these projects remains limited at the global level. In Busch et al. (2022) the authors review policy studies addressing the cement and concrete sector and their results show that high cost is the main barrier for the sector in 65% of the articles evaluated. These data demonstrate a policy that stimulates market competitiveness, guarantees legal security for investors, and dialogs with the specific characteristics of each industrial process.

Preliminary conclusions: This study shows that the climate emergency has been included in the agenda of several policymakers in the international context, who have been trying to address the specific demands of each industry sub sector in order to meet the neutralization targets. The results of the systematic literature review revealed that each industry sector has its own unique challenges and opportunities when it comes to reducing emissions. By tailoring climate policies to specific sectors, policymakers can address sector-specific barriers and leverage opportunities for emission reductions. The papers generally suggest that the economic aspect and the lack of incentives for the development of capital-intensive technologies have been an important barriers to project scalability and demand attention from governments in creating strategies to address these issues. The steel sector plays a key role for decarbonization goals. The cap and trade mechanism, or carbon market, is pointed out in the literature as a solution for the sector, but it highlights the need for policies that determine the use of renewable energy for plants, the reduction of the use of mineral coal and subsequent incentive to use compressed woody biomass to prepare metallurgical coke, stronger energy efficiency standards and stimulate demand for green steel. For the cement sector, the papers highlight the need to adopt clean technologies,

improve energy efficiency and promote the use of alternative materials and fuels with lower carbon intensity. The adoption of policies that involve the entire value chain of this industry and incentives for CCU technology may be paths that bring positive results in the long term. In the case of the articles dealing with the Energy-Intensive Industrial (EII) sector, it was found that the authors provide a macro view of the incentive mechanisms currently used and make a critical reflection on them. Some authors differ on the effectiveness of the carbon market, depending on market behaviour, and advocate solutions by looking at the technological aspect of each industry. Encouraging the stimulation of technologies involving CCU is recurrently cited among sectors and pointed out as a crucial factor to be incorporated in sectoral policies. Therefore, new policies for climate change in a new decade are essential to tackle the escalating crisis, limit global warming, foster global cooperation, leverage technological advancements, seize social and economic opportunities, and respond to evolving public awareness.

Yuri Souza Beleli
Universidade de São Paulo (USP)

Abstract Title: Optimization of a continuous temperature swing adsorption system for gases originated from biomass combustion

Authors' Names & Affiliation Institutions of all authors (in order for publication): Yuri Souza Beleli (USP), Galo A. C. Le Roux (USP), José Luis de Paiva (USP), Marcelo Martins Seckler (USP)

Abstract: Post combustion carbon capture has been shown to be an important process for mitigating the negative effects of greenhouse gas emissions. Implementing a temperature swing adsorption (TSA) system employing fluidized beds for the removal of carbon dioxide of gases is a promising method for reducing emissions, and when trying to bring this technology from the academic environment to the industrial scope it is necessary to evaluate its cost and how that will influence in the system operation. From the operational cost of heat and pressure management to the capital cost of the system itself, it is necessary to study how this system can be accomplished while minimizing its overall cost and energy consumption. The system is composed of an adsorption and a desorption column, with counter-current flow, in which the solid flow (adosrbent zeolite 13x) descends and the gas flow ascends. The solid flow is continuous as it goes through both columns so that the carbon dioxide can be adsorbed and then desorbed for capture. The system was optimized using a 3-stage adsorber and a 3-stage desorber, with heat-exchangers that can be used in each stage and in the gas feed of both

columns. The constrained variable in the adsorption column is the solid-to-gas mass feed ratios. The pressure loss in the system was determined utilizing the minimum fluidization velocity and compressors were added to compensate it. The system variables were studied modifying the desired setpoint for the product gas (lean in CO2) and it was shown that higher removal of CO2 determines that the system cost will also be higher, as it will demand more heat management. It was found that substantial CO2 recovery with 98% purity can be achieved and that the heat load in the desorption column accounts for the largest part of the energy optimized cost in the process. This study shows which aspects of the system are most important when determining its cost, so that when it is industrially applied, practical solutions may be considered to reduce the cost even further.

Keywords: Fluidized Bed, Optimization, Adsorption, Carbon capture, Temperature Swing Adsorption.

Introduction and Objectives: In biomass combustion processes for energy production, the capture of CO2 is of great interest, as it is possible to reduce the effects of the emission of this gas into the atmosphere. Adsorption is an exothermic process, while desorption is an endothermic process. This makes the former favourable in reactors with low temperatures, while the latter is favoured in reactors with high temperatures. A studied method for post-combustion carbon capture is the Temperature Swing Adsoprtion, which defines that the continuous system composed of the two parts (adsorption and desorption) should be operated at temperatures that favour their respective mechanics, thus modulating the temperatures between them. The objective of this research is the development of models to be optimized to enable the large-scale implementation of adsorption technology for post-combustion CO2 capture from biomass. These models are implemented to reduce the cost of the system, thus being able to study how the system variables will influence in its economic aspects.

Methodology: For the system to be evaluated and optimized in the area of interest, it is necessary for it to be mathematically described, highlighting the variables, their meanings, and the equations that relate them, translating the physical process into a system of equations. After representing the system with its equations, such as adsorption equilibrium, mass and energy balances and adding heat exchangers and compressors, the system was optimized in order to minimize its cost. The optimization was carried out in GAMS as an MINLP. After the optimization, the results were discussed and evaluated so the system variables importance for its cost could be studied.

Preliminary results: With the equilibrium simulations it was possible to determine that to efficiently remove the CO2 in the studied gas a number of stages in the columns of the system bigger than 2 and lesser than 5 would be required (with heat management) and that the temperature in the stages, as well as the available solid (adsorbent) flow, would be the determining factors when managing the adsorption equilibrium. For the operational cost of the heat exchangers, it was determined that a more efficient removal of CO2 states that a bigger

cost will be required and that most of this cost derives from the heat management of the desorption column. When studying the capital cost of the heat exchangers, it becomes evident that not all stages of the columns need heat exchangers and that the heat management of the columns do not need to be applied in all parts of the system, as there will be heat exchange between the solid and gas flow, as well as the heat added or subtracted due to the adsorption and desorption processes.

Preliminary conclusions: Heat management has been determined as the biggest contributor of the cost of the system. The optimization algorithm designed makes it so the system can be studied with a number of variations, when intended to be applied in similar TSA systems. That leaves the floor open to alternatives to reduce the cost even further, as it is possible to study alternative energy sources so that the heat management cost can be reduced. When utilizing fluidized beds, it is also necessary to manage the pressure drop costs that will be directly influenced by the solid and gas flow and its minimal fluidization velocity, which will change depending on the characteristics of the deployed adsorbent (in this case zeolite 13x). This study reinforces that TSA can be utilized as a promising carbon capture technology and that it is viable and economically accessible.

SHORT ORAL SESSION E

9/11 10h10 - Short Oral Session E

0911 – ETE6 (TV1)

Chairs: Virginia Parente – Suani Coelho

Thiago Giancoli Berto
Escola Politécnica of the University of São Paulo (Poli-USP)

Abstract Title: Green and Yellow Hydrogen: from the federal fiscal war to global value chains

Authors' Names & Affiliation Institutions of all authors (in order for publication): Thiago Giancoli Berto, Escola Politécnica of the University of São Paulo / Denis Cristian Alfonte Lupaca, Escola Politécnica of the University of São Paulo.

Abstract: Critical exposition of "Green and Yellow Hydrogen" initiatives led by Brazil, accompanied by the rearrangement of federative entities and the country itself in Global Value Chains.

Keywords: Hydrogen; Green Hydrogen; Green and Yellow Hydrogen; Tax War; Global Value Chain (GVC); Decarbonization; Energy Transition; Brazil.

Introduction and Objectives: The name “hydrogen” derives from the Greek “hydro” and “genes”, which means “water generator”. It is considered, to this day, an alternative fuel, energy vector and energy carrier. It has a calorific value of 141.9kJ/g, which is approximately 4.8 times greater than that of ethanol (29.7kJ/g) (NANDA et al., 2017). However, hydrogen (H2) can also be an “ethanol generator” – it would be “Green and Yellow Hydrogen” (H2VA) –, through the process of thermal or steam reforming (among others, advantageous, since the first is more energetically dense than the second). Given the competitive and sustainable condition that ethanol has historically acquired in Brazil, and in light of the Sustainable Development Goals (SDG's), the conversion of this alcohol into hydrogen, based on extensive national scientific and technological development, can make H2, in addition to no longer being seen as an alternative fuel to becoming a reference, making Brazil a protagonist in the scenario of decarbonization of the Economy and energy transition. The perennial search for valuing the terms of trade is one of the roles of a Nation-State. An improvement in the relationship between the prices of a country's exports and imports – "ceteris paribus" – allows for an increase in the population's real income and, consequently, an improvement in quality of life. To this end, the addition of value to products produced in a territory is conditioned, accompanied by the (inherent) increase in tax revenue and the complexity of the means and methods used to deliver

the goods to the customer or user. The energy transition can be understood as a Brazilian brand (EPE, 2022). Well "c." 14% of the energy matrix comes from renewable and clean sources, while, worldwide, this figure is made up of 2%. Thus, in addition to improving this distinction, Brazil (and its federative entities) can position themselves as important drivers of change in the structure and set of sources used in global energy generation. In this context, hydrogen plays a fundamental role. The present work aims to estimate Brazil's insertion in global value chains (GVCs) based on the pioneering development of H2VA. Furthermore, it is proposed to analyse internal characteristics relating to Brazilian states, as well as locational factors, technological overflow and absorption capacity (RIBEIRO; GONÇALVES; FREGUGLIA, 2013), aimed at the installation of industrial plants in them, and the entire production chain which supports the energy transition enabled by hydrogen, as well.

Methodology: As a methodology to achieve the objectives of the work, a review of specialized literature was carried out, and the main reference was a recent article from the "Revista Brasileira de Energia", called “Brazilian Hydrogen Economy Development”, authored by Sabrina Macedo, Drielli Peyerl and Donato da Silva Filho. The proposal was to use the SWOT analysis carried out by the authors as a subsidy, in order to problematize it, and direct the examination proposed here to hydrogen from ethanol – H2VA –, in the Brazilian context, internal and external. To this end, a “Relevance” index was assigned, in addition to the four aspects established by the matrix: “Strengths” and “Weaknesses” – as internal factors – with “Opportunities” and “Threats” – as external factors. “Hydrogen from ethanol” was classified as “Opportunity”, and assigned relevance “5”, on a scale of 3 to 9. In the comparison with “Strengths” and “Weaknesses”, it performed better when crossed with “Competitiveness of variable renewables”, due also to its relevance (index 9). The worst performance was in “No specific regulation”.
Based on these data – with emphasis on these extremes – it is suggested to expand the discussion of its causes and consequences for the technology developed and improved on Brazilian soil. Adding the layer of the “fiscal war”, which has been waged by states and municipalities to encourage the production of hydrogen that is still only green (H2V), and the creation of hubs capable of promoting the reindustrialization of the country (AHK, 2023).

Preliminary results: As “Strengths”, the following were considered: “international partnerships”, “'Programa Nacional do Hidrogênio' (PNH) pillars to develop a hydrogen Economy", “Resolutions of the 'Conselho Nacional de Política Energética' (CNPE) for hydrogen development" and “Competitiveness of Variable Renewables”. For “Weaknesses”, the following were listed: “Technological and Cost Challenges”, “Incipient Natural Gas Market”, “Institutional, legal and regulatory structures must be improved” and “No Specific Regulation”. Currently, more than 95% of the hydrogen consumed in the world is extracted from fossil fuels, mainly natural gas, through the action of superheated steam. Metallic catalysts are used to facilitate chemical reactions, such as those from the platinum mineral group, which creates bottlenecks. If, on the one hand, with hydrogen, the concentration of energy resources

tends to decrease, on the other, more than 90% of iridium, the main representative of the group, is concentrated in a single country, South Africa (PEREIRA, 2023).

The ethanol distribution network could be used to implement H2VA in the mobility sector, greatly facilitating the implementation of charging points such as those required for conventional electric cars. Once the "Strengths" have been ratified, suggestions for an approach to overcoming the "Weaknesses" highlighted are now proposed. The "Research Centre for Greenhouse Gas Innovation" (RCGI), based at the University of São Paulo (USP), with support from the São Paulo State Research Support Foundation (FAPESP) and Shell, develops, according to the Ministry of Finance, the "most advanced project in the area of ecological transformation in Brazil". With H2VA as its vector, it plans, for the beginning of next year, the first renewable hydrogen station based on ethanol in the world (JORNAL DA USP, 2023). Therefore, also counting on the partnership of companies such as Toyota do Brasil, Raízen and Hytron, we are moving towards solving technological and cost challenges. Of national Engineering and intellectual property, active, communes and integrates from the University to Industry and Government actors (ETZKOWITZ, 2017). A "gap" occurs in existing technical professional training. This situation of lack of qualified human resources, both at operational and Engineering and Technology levels, condemns the country to depend, until this changes, on international suppliers (MACEDO; PEYERL; FILHO, 2023).

In relation to hydrogen hubs, the Port of Pecém is leading the race. This port complex in the state of Ceará builds its business model based on leasing land within an export processing zone (ZPE), which offers tax advantages. Its proximity to Europe, on the "corner of Atlantic". Envisioning the articulation with H2VA, the northeast would have the capacity to supply ethanol (and freight discounts to Pecém), only from September to March. From April to November, the sugar cane harvest takes place in the
Center-South.

Preliminary conclusions: The most abundant chemical element in the Universe, Hydrogen is mostly associated with other atoms in the constitution of molecules other than the simple pure substance Hydrogen. Green and Yellow Hydrogen, by providing the genesis (as it has in the name) of not only an energy alternative and an upgrading perspective in GVC's for Brazil, can perhaps give this element the impact on human activities, to the same extent as its abundance. The energy transition can be understood as a "becoming aware".

There are several strategies that contribute to the increase in the characteristics that are delivered – and perceived by them – to the consumer, which is conceptualized as "value". According to Astute Analytica (2023), the global hydrogen market is estimated to increase revenue from US$206.6 billion in 2022 to US$761.3 billion by 2040. However, much more than scaling processes in order to mitigate costs, there are clear chances of "promoting the inclusive development of Brazilian society in the process of developing this market, from economic and educational aspects, also considering those related to the fiscal aspect" (MACEDO; PEYERL; FILHO, 2023).

It is intended, in results and conclusions subsequent to the Preliminaryies presented in this

work, to estimate, with indices, the social impact and generation of positive externalities to Society – as a vector of social transformation – of "deep tech" ventures such as H2VA, the evolution along the TRL (Technology Readiness Level) scale and public understanding of the transformations involved (a Porter diagram can assist in the analyses). A Hydrogen Economy and Diplomacy is inaugurated. And, if we want, "development on a human scale", 40 years after it was proposed (MAX-NEEF, 1983).

Melodie Kern Sarubo Dorth Sinegalia
Graduate Program in Planning and Use of Renewable Resources, Federal University of São Carlos, 18052-780, Sorocaba, São Paulo, Brazil

Abstract Title: Methodology Proposal for Control Point Surveys: Considerations In The Context Of Remote Forest Monitoring With Emphasis On Carbon Stock

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Abstract: Assessing carbon stock in forest ecosystems is a critically important task in times of climate change, as it is one of the key tasks in understanding and forecasting the impacts of these changes. It also plays a vital role in the development of tools and policies aligned with carbon mitigation and adaptation strategies. Ecological indicators are pivotal in this context, providing valuable insights into ecosystem dynamics and the carbon sequestration capacity of vegetation. In this context, remotely piloted aircraft systems (RPAS) have emerged as a promising technology, enabling the acquisition and analysis of various forest indicators through the combination of products and techniques. One of the most relevant ecological indicators for estimating carbon stock is tree height, as it is not only related to ecological diversity but also serves as a critical indicator of forest structure. Taller trees generally have more wood volume and, consequently, more carbon. However, limitations exist concerning the positional accuracy of these products, especially in areas with dense vegetation. It is common practice to adopt ground control points (GCPs) in adjacent areas to the forest to minimize these effects. These points are obtained through surveys using Global Navigation Satellite Systems (GNSS) receivers. The primary benefits include the correction of geometric distortions and the enhancement of spatial accuracy in planimetric aerial images. Nevertheless, challenges persist, particularly concerning the altimetric component's accuracy. Moreover, there is a scarcity of

studies assessing the accuracy of the results. In this research, with the aim of providing a replicable methodology for obtaining GCPs in forest environments with the highest possible accuracy, particularly in the altimetric component, we conducted surveys using GNSS receivers at points within a pre-established high-precision planimetric network in the municipality of Buri, São Paulo, with coordinates validated and adopted as ground truth for accuracy analysis. The Spectra SP60 receiver by Trimble was employed in five different positioning techniques, encompassing both relative and absolute methods, along with their respective processing methodologies. Based on the findings, we hope to formulate an optimal methodological protocol in terms of cost-effectiveness for obtaining accurate GCPs in forest environments. Our aspiration is that the results of this study will provide significant contributions to the development and enhancement of tools aimed at formulating strategies related to the assessment of carbon stock in forest ecosystems.

Keywords: Global Positioning System; GPS; Precision; Accuracy; Altimetry; Carbon.

Introduction and Objectives: While unprecedented climate changes are occurring on a global scale, primarily due to human-caused carbon emissions, preserving forests and understanding forest dynamics have become paramount. Remote sensing stands out as a powerful tool for monitoring these ecosystems, providing products for analysis, synthesis, and reporting that contribute to informed decisions, enabling sustainable planning and management (Gómez et al. 2019).

Currently, there is a trend in using LiDAR to map trees at landscape scales; however, such surveys require expensive aircraft and specialized sensors, whereas RGB images can be obtained economically. Moreover, coupled with the recent availability of RPAS, commonly known as drones, it has enabled the generation of photogrammetric products with an unprecedented level of detail and ease (Mlambo et al. 2017). The significant potential of these platforms has motivated a wide range of applications in forest monitoring and its structure, including obtaining measurements such as tree height and crown diameter (Pourreza et al. 2022). However, a challenge is associated with the presence of errors in the accuracies obtained from these products, particularly in the altimetric component. To minimize these effects, it is common to adopt strategically distributed points in the area to be mapped, enabling their identification in the generated images (Singh et al., 2023). In surveys aimed at producing small-scale forest restoration interventions or monitoring changes over time, their inclusion is considered essential, playing a crucial role in the validation and correction of photogrammetric products and in the georeferencing of the point cloud (Swinfield et al. 2019). These points are commonly referred to as GCPs and can be either permanent ground features or reference targets placed on the ground before the flight. Their three-dimensional positions are usually obtained through surveys using GNSS receivers. Despite the high precision provided in the planimetric component, GNSS has limitations in the altimetric component (Pourreza et al. 2022). Another factor relates to accuracy, as manufacturers typically present achievable precision levels but do

not mention the relevant accuracy associated with them. In this study, aiming to provide a methodology for obtaining GCP coordinates with the highest possible accuracy, we conducted surveys using GNSS positioning techniques in a previously established planimetric-altimetric network. The control points were selected to provide conditions similar to the GCPs used in the context of remote forest monitoring, along with vertices in 'ideal' situations for comparison. Based on the results obtained, we hope to develop a methodology protocol that offers better cost-effectiveness in terms of data collection time, type of receiver, and achieved accuracy, contributing to the development and improvement of tools aimed at formulating strategies related to the assessment of carbon stock in forest ecosystems.

Methodology: This study has been divided into stages, taking into account the survey and processing techniques commonly employed in GCP (Ground Control Point) surveys, both for absolute and relative positioning. Subsequently, we will proceed with the analysis of the obtained results. Based on these findings, our aim is to develop a protocol for obtaining GCPs in a forest environment, with the goal of achieving the highest accuracy attainable through such a protocol.

Step 1: Surveys Using Relative Positioning Techniques

Surveys were conducted using the Real Time Kinematic (RTK), relative static, and relative static-rapid (also known as stop-and-go) methodologies, employing various tracking times at control points with minimal forest coverage or in adjacent areas to the forest. The base receiver was positioned at a control point designated as Cepegeo01 (abbreviated as CP01), while the rover traversed the selected control points, following the previously mentioned criteria.

Subsequently, the data underwent processing and adjustment. The data from the Brazilian Continuous Monitoring Network were utilized for base processing in Survey Office and Topcon Tools software. Subsequently, the rover data were processed using the same two software tools.

Step 2: Surveys Using Absolute Positioning Techniques

Surveys were conducted using the Precise Point Positioning (PPP) and Single Point Positioning (SPP) methodologies, employing various tracking times. Subsequently, we will process and adjust this data using the Brazilian Institute of Geography and Statistics (IBGE) website, referred to as PPP - Online Service for GNSS Data Post-Processing.

For SPP, we will utilize the downloaded (unprocessed) data in Topcon Tools and Survey Office.

Step 3: Data Tabulation and Analysis

In this stage, after tabulating the obtained results, we will draw conclusions and perform an analysis of the accuracies achieved for each method/tracking time. The goal is to assess which method performed the best, comparing the GCPs in a forest environment to the control points installed in an ideal situation.

Step 4: Protocol Development

In this stage, we will develop the protocol that is the main objective of this study. The aim is to guide future studies in obtaining GCPs with a focus on the relationship between accuracy, methodology, and tracking time.

Preliminary results: Step 1 was carried out at 9 selected control points, following the previously mentioned criteria. Among these points, CP01 and CP20 are in what can be considered an ideal situation, CP02 and CP10 are located in areas with higher forest density, and CP08 and CP09 are adjacent to the forest with low forest coverage.
The Z coordinates obtained for the stop-and-go relative positioning technique are presented in Table 1, where the column labeled Zref (Reference Z) corresponds to the homologated coordinate in the mentioned network, and the column Zsag represents the coordinates found for the control points when the stop-and-go technique was employed.

Point Z ref Z sag
CP01 633,832 633,739
CP20 632,524 632,439
CP03 633,134
CP04 632,924
CP05 633,3
CP06 634,126
CP07 639,182
CP08 640,865 640,335
CP09 641,285 641,823
CP11 641,988
CP12 641,805 641,453
CP10 642,1 641,431
CP02 642,435 641,662
CP13 641,882 641,399
CP14 640,236 639,62

Preliminary conclusions: The points positioned in locations considered ideal (without signal interference or obstacles) achieved a positional accuracy better than 10 cm using the stop-and-go method. In contrast, the points located in areas with forest coverage exhibited discrepancies of up to 80 cm for vertices with higher coverage and 50 cm for adjacent vertices.
These significant altimetric errors have substantial implications for RGB image processing. They compromise georeferencing, orthorectification, the accuracy of 3D models, visual consistency, and height-related metrics, resulting in inaccurate results that hinder the utility of

the images for subsequent analyses.
Minimizing height errors during field data collection is crucial to ensure the attainment of reliable and accurate results. We are currently implementing new adjustment methodologies to assess whether there are improvements in the coordinates obtained and developing the methodological protocol based on the results obtained.

Mateus Castagnet
University of São Paulo

Abstract Title: Carbon Footprint Reduction through the Replacement of LPG with Biodigesters: A Case Study
Authors' Names & Affiliation Institutions of all authors (in order for publication): Mateus Castagnet

Abstract: This scientific article addresses the issue of reducing the carbon footprint through the replacement of liquefied petroleum gas (LPG) with biodigesters in the context of residential installations. The research was based on a case study that evaluated the impacts of transitioning from LPG to a residential biodigester model, developed by a study from the Escola Politécnica da Universidade de São Paulo. Biodigesters, systems that convert organic waste into biogas, were implemented as a clean and renewable alternative to meet the cooking and hot water needs of the community. The main objectives of the study were to quantify the reductions in CO2 emissions, the economic and environmental benefits resulting from the implementation of biodigesters, and to analyse the challenges associated with the adoption of this technology. The results demonstrated a significant decrease in CO2 emissions after the replacement of LPG with biodigesters. This occurred due to the capture of methane released during the decomposition of organic waste, which would otherwise have contributed to global warming. Furthermore, biogas production also reduced the community's dependence on fossil fuels, resulting in long-term financial savings. However, the research identified important challenges, such as the need for community awareness and training to operate and maintain biodigesters efficiently. Additionally, the availability of suitable organic waste for biogas production and the necessary infrastructure for biodigester deployment are important considerations to be addressed.

Keywords: Residencial, biodigester, CO2, emissions.

Introduction and Objectives:
Introduction: In a world grappling with the urgent need to combat climate change and reduce greenhouse gas emissions, the search for sustainable alternatives to conventional fossil fuels has become paramount. One such alternative gaining attention is the replacement of liquefied petroleum gas (LPG) with biodigesters in residential settings. This scientific article delves into the potential of biodigesters to significantly reduce the carbon footprint associated with residential energy consumption. Through a comprehensive case study, we explore the

environmental and economic implications of this transition while shedding light on the challenges and considerations involved.

Objectives: As the world grapples with the imperative to mitigate climate change, the findings presented in this research underscore the importance of embracing clean and renewable technologies like biodigesters. These technologies not only offer a pathway to reduce carbon emissions but also contribute to a more sustainable and environmentally conscious future. It is our hope that this study will serve as a catalyst for wider adoption and investment in such environmentally friendly alternatives, promoting a healthier planet for generations to come.

Methodology: The study conducted by Ronan at Poli-USP, which focused on the development of residential biodigesters sized to meet the needs of an average family of four, provided a unique opportunity to quantify the significant reduction in carbon emissions when replacing liquefied petroleum gas (LPG) with biogas.
The research initially assessed methane emissions released during the decomposition of organic waste in the biodigesters. This analysis revealed that methane, a potent greenhouse gas, was effectively captured and converted into biogas instead of being released into the atmosphere. This resulted in a remarkable reduction in direct methane emissions.
Furthermore, the study considered emissions associated with the production of LPG, from oil extraction to transportation and refining. These emissions, often underestimated, are a significant part of the LPG lifecycle and contribute to the carbon footprint of the fuel. The direct comparison of these emissions with the emissions reduced by using biodigesters showed substantial carbon savings.
While specific results may vary based on factors such as the composition of organic waste, climatic conditions, and the LPG production process, Ronan's study demonstrated that replacing LPG with biogas in households has the potential to result in a significant reduction in carbon emissions. This not only contributes to climate change mitigation but also promotes a more sustainable and environmentally responsible approach to residential energy supply.

Preliminary results: Our initial findings from the study conducted at Poli-USP, focusing on the substitution of LPG with biogas in residential settings, show promising results. The research indicates a significant reduction in carbon emissions. This reduction is primarily attributed to the effective capture of methane emissions during organic waste decomposition in biodigesters and a thorough lifecycle analysis of LPG emissions. While these preliminary results are encouraging, further data analysis and research are necessary to provide a comprehensive assessment of this transition's environmental and economic impacts. Nonetheless, this research highlights the potential of biogas as a sustainable energy alternative in mitigating carbon emissions associated with residential energy consumption.

Preliminary conclusions: In conclusion, the replacement of LPG with biodigesters has proven to be a viable strategy for reducing the carbon footprint in communities, providing significant economic and environmental benefits. However, it is essential to consider awareness, training,

and adequate infrastructure as key elements for the success of this transition. The study underscores the importance of promoting clean and renewable technologies as part of a global effort to combat climate change and promote environmental sustainability.

Leonardo de Freitas
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Abstract Title: Economic viability of hydrogen

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Abstract: According to Bloomberg NEF, global financing commitments for the sector through 2030 totalled $146 billion as of December 2022, a 46% increase since BNEF's previous update in January 2022. Globally, total energy spending clean services reached US$1.1 trillion in 2022, led by China at US$546 billion, followed by the EU (US$180 billion) and the US (US$141 billion). In the US, the surge in interest is embodied in three major pieces of legislation — the Infrastructure Investment and Jobs Act of 2021 (also known as the Bipartisan Infrastructure Act), the Chips and Science Act (CHIPS Act), and the Inflation Reduction Act (IRA) from 2022. Not only did the EU quadruple its 2030 target for renewable hydrogen supplies, but the US also walked away with one of the most generous green hydrogen subsidies in the world through the IRA. Other countries are also very much in the clean hydrogen race, including China, given its overall leadership in clean energy and significant spending on electrolyser capacity, far exceeding predictable demand. Australia, Chile, India and Japan are also involved, as well as some of the world's leading oil exporters in the Middle East, where Saudi Arabia and the United Arab Emirates have enhanced their already robust plans to be the world's leading hydrogen exporters in some capacity. (including blue and green ammonia). Momentum has been building, and 2022 in February, the world's first shipment of liquid hydrogen left Australia for Japan. In August, the first hydrogen-powered commuter trains were commissioned for full time service in Germany. Just before the end of the year, the world's first project for industrial-scale hydrogen power, the HYFLEXPOWER project, completed its initial trials in France, using hydrogen mixed with natural gas in a 30:70 volume mix for power generation.
According to the International Energy Agency (IEA), global hydrogen demand in 2030 will occur mainly in the industry sectors with approximately 100Mmt, Grid Injection 50Mmt, ammonia-fuel 20Mmt and synfuel 20Mmt.

According to Bloomberg NFE, electrolysis production capacity in 2030 will be mainly in China and Europe, with approximately 75GW each, while the United States and Canada with 50 GW, and Australia with 30GW.

Keywords: Hydrogen, scalability, demand, investment, subsidies, legislation, Tax Credit.

Introduction and Objectives: Hydrogen can be stored longer and more efficiently as a last-resort replacement for renewables such as wind, solar and hydropower than utility-scale batteries; and because it burns at high temperatures, it can be a clean substitute for coking coal. Hydrogen, however, faces scalability issues in creating electrolyzers, leakage issues (when it comes to pipelines and storage), and cost hurdles, along with "not-in-my-backyard" (NIMBY) hurdles. The high cost of scalable projects has certainly slowed down the development of hydrogen projects globally. But signs of progress have emerged in recent years. This stems in part from a general acceleration in investments in green technology, which Bloomberg NEF (BNEF) indicates has reached $1.1 trillion with 30% funding growth in 2022. While very little of this acceleration has been in hydrogen, The start of 2023 brought the first large-scale global hydrogen financing with an $8.5 billion hydrogen project in Saudi Arabia.
Between 2021 and 2022, the US enacted a series of new laws, including the Reducing Inflation Act, which, together with previous legislation and existing authorities, are expected to provide up to $1.7 trillion in investment incentives. A significant proportion of these incentives are for hydrogen projects, including through support at hydrogen hubs across the country. The tax credits provided by the Inflation Reduction Act are so generous that the net costs of producing green hydrogen after adjusting for tax benefits could be negative by the end of this decade. In response, Europe has enacted its own Green Deal Industrial Plan, and government incentives are being offered in a growing list of countries already endowed with renewable resource potential and/or with the incentives to reach net zero, including Australia, Chile, China (the world's leading hydrogen producer), India, Japan, Oman, Saudi Arabia and the United Arab Emirates.

Methodology: Global hydrogen demand by 2030 could range between 103 million metric tons per year (MMt/year) and 200 MMt/year if the world is on track to achieve net-zero emissions by 2050, above 94 million metric tons (MMt) in 2021, according to the International Energy Agency (IEA),
Bloomberg NEF and the Hydrogen Council.

Some analysts project growth to accelerate after 2030, reaching about 500 MMt/year to 660 MMt/year by 2050. In addition to its traditional use in the refining and chemical industries, hydrogen is making inroads in sectors such as steel production, power generation/energy storage and transportation. For example:
• On the industrial side, the world's first fossil-free steel has already been delivered to Sweden.
• On the energy side, the US Clean Energy Advanced Storage centre could be generating power by 2024 through an 840 megawatt (MW) gas turbine burning a mix of 30% green hydrogen and 70% natural gas. • On the transportation side, while hydrogen fuel cell electric vehicles

(FCEVs) remain a much smaller market than battery EVs (BEVs), the number of FCEVs on the road reached more than 51,000 at the end of 2021, a 50% increase year over year, with promise in heavy trucks and passenger vehicles.
Investments are also increasing. Investments in clean hydrogen will likely triple year over year in 2022, albeit from a low base, with the majority focusing on electrolysers, according to Bloomberg NEF. • Of the $1.111 billion in clean hydrogen investment in 2022, 99% went to electrolysers, while hydrogen pipelines, underground storage and thermochemical hydrogen production projects together received just over $13 million.
• Correspondingly, global electrolyser shipments surpassed 1 gigawatt (GW) in 2022, more than doubling from 2021, and could again double or even triple in 2023, driven by demand from China, Europe and Australia.
However, rising interest rates and recent banking sector troubles could pose some challenges, especially for cleantech startups.
On the other hand, the formidable subsidies and other support mechanisms available through the Bipartisan Infrastructure Act, CHIPS and IRA legislation in the US, as well as the European Industrial Plan Green Deal and Net Zero Industry Act (both adopted in the first quarter of 2023), could actually support increased private equity investment as well as sustainable debt issuance.
•According to IEA and BNEF, the costs of Alkaline Electrolysers could fall quickly this decade, thanks to investment and scalability in this area. From 1000 USD/KW (2022) to 400 USD/KW in 2030, and 200 USD/KW in 2040.
• According to the IEA and BNEF, 80% of costs will already be reduced by 2026 in the United States for Proton Exchange Membrane Electrolysers. With a cost of 200 USD/KW in 2035.

Preliminary results:
•LCOH designed for gray, blue and green hydrogen (powered with dedicated solar) in the US without tax credits:
Green Hydrogen – 4.5 $/KG in 2022, 3 $/KG in 2025, 2 $/KG in 2030
Blue Hydrogen – 1.5 $/KG constant
Gray Hydrogen – 1.0 $/KG constant

•LCOH designed for gray, blue and green hydrogen (powered by dedicated solar) in the US with tax credits:
Green Hydrogen – 2.0 $/KG in 2022, 0.5 $/KG in 2025, -0.5 $/KG in 2030
Blue Hydrogen – 0.5 $/KG constant
Gray Hydrogen – 1.0 $/KG constant

(Note): Assuming natural gas price of US$3 per million British Thermal Units (MMBtu)
Source: Citi Research Estimates
(Note): LCOH – (Levelized Cost of Hydrogen)

•Production Tax Credit (PTC) and Investment Tax Credit (ITC) for Clean Hydrogen Offered by the Inflation Reduction Act (IRA)

Life Cycle GHG Emission Rate (kgCO2/kgH2) < 0.45

Basic interest rate: PTC ($/KgH2) = 0.6; ITC = 6.0%

Increase in Credit Value When Conditions Are Met: PTC ($/KgH2) = 3.0; ITC = 30.0% Qualified Hydrogen Types (estimated): Blue hydrogen with >=95% carbon captured; or green hydrogen

•LCOE (Levelized cost of electricity) designed for US utility Solar Photovoltaics, taking into account ITC before and after IRA implementation

Before: $25/MWh in 2022, $30/MWh in 2025, $25/MWh in 2026, $25/MWh in 2030 After: 25 $/MWh in 2022, 20 $/MWh in 2025, 20 $/MWh in 2026, 15 $/MWh in 2030

•LCOE (Levelized cost of electricity) designed for US Onshore Wind Farms Taking into Account PTC Before and After IRA Implementation

Before: $30/MWh in 2022, $29/MWh in 2025, $25/MWh in 2026, $25/MWh in 2030 After: 20 $/MWh in 2022, 15 $/MWh in 2025, 12 $/MWh in 2026, 10 $/MWh in 2030

Preliminary conclusions:
USA: Tax credit expected to lead to negative costs of green hydrogen, even before 2030
Currently, blue hydrogen yet enjoys cost advantages over green hydrogen in the US.This is due to the availability of cheap natural gas as well as tax benefits including the 45Q CCUS tax credit and the clean hydrogen production tax credit (PTC).

• Our projected LCOH predicts that blue hydrogen will lose its advantage to green hydrogen starting in the mid-2020s. In fact, the LCOH of green hydrogen could fall below zero even before 2030, after accounting for credits taxes on renewable energy and the production of clean hydrogen. • The IRA approved in August 2022 provided increased tax credits for blue and green hydrogen. For the first time, it provides clean hydrogen tax credits of up to $3 per kilogram of qualifying hydrogen. • Most importantly, clean hydrogen production plants will be able to benefit from accrued tax credits if the hydrogen is produced by electrolysis of water powered by renewable electricity. • The legislation also expanded and increased existing investment tax credits (ITC) and PTC for renewable energy, including solar and wind, as well as 45Q tax credits for CCUS.

Of the two main components of green hydrogen extending the ITC/PTC to future solar and wind projects would further help reduce the LCOE (Levelized Cost of Electricity) of renewables, accelerating deflation of the total cost of green hydrogen, as electricity costs could represent 50%-70% of LCOH (Levelized Cost of Hydrogen) by 2030.

• Now, new solar projects that begin construction by 2033 can claim a 30% ITC, leading to a discount of around 25% on solar LCOE.
• Similarly, PTCs (Production Tax Credit) for wind developers, which expired at the end of 2021, are now extended until at least 2033, potentially reducing wind LCOE by up to 70%.

Signed in November 2021, Bipartisan Infrastructure Act (BIL) allocated a total of US$9.5 billion for R&D (research and development) and demonstration of clean hydrogen. Specifically, $8 billion is directed toward the region's clean hydrogen hubs, where clean hydrogen producers, consumers, and connective infrastructure are located in close proximity.

The CHIPS Act became law in August 2022. The law authorized up to $12 billion for R&D for the Department of Energy, including for the Advanced Research Projects Agency-Energy (ARPA-E) working on advanced CHIPS technologies energy, including hydrogen.

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Abstract Title: Business Models for the Brazilian Natural Gas Market in Times of Energy Transition and National Deregulation

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Abstract: The Brazilian natural gas market is developing and opening to a free market. It is becoming essential to develop and apply innovative business models with characteristics specific to the country that can follow and respond to trends in the global energy transition based on the decarbonization of energy sources. It must prioritize and promote competition in the sector. Therefore, lessons are to be learned from the experience of mature international markets. Therefore, this work aims to map business models for natural gas in developed markets, which can respond to the gaps faced towards a low-carbon energy transition, such as how Brazilian companies can operate in the market in an environmentally sustainable way. Furthermore, the market will evolve economically to meet energy transitions and Brazilian deregulation.

Keywords: Natural gas; Business Models; Energy transition; Deregulation; Brazil.

Introduction and Objectives: Since 2012, the Brazilian natural gas sector has undergone organizational changes, amalgamated mainly by introducing new legal and regulatory instruments that promote market opening processes and encourage greater competition in the sector. This fact implies, for all economic agents involved, revisiting strategies, and developing and applying innovative business models aligned with new organizational structures, but without losing links with the country's own characteristics. Such reviews are essential for gas markets to advance in the country and for natural gas to respond to the demands and trends of the energy transition, which are imposed on a global scale, towards the decarbonization of nations' energy matrices. Lessons can be learned from experiences observed in more mature international gas markets. Many of these lessons must be adequately adapted to current Brazilian realities. Therefore, this work aims to systematically map business models for natural gas in more developed markets, evaluating them as innovative proposals that can be adopted in Brazil. Cases from European and American countries will be analysed regarding the moment markets developed and how it was seen and practiced by companies and governments when drafting their legislation and regulations.

Methodology: The dimensions to be analysed are classified into main thematic axes, with the following contents: (a) political and social, (b) economic, (c) legislative and regulatory, and (d) technical and environmental. These dimensions were chosen because they cover all impacts directly related to the natural gas market. It is understood to analyse the main impacts of the business models to be selected in promoting natural gas as an essential vector in energy transition processes. The models will be tested considering recent events in global geopolitics, especially the war between Russia and Ukraine, which has impacted the future visions of important nations regarding the sustainable role still reserved for natural gas in energy transitions.

In this sense, the following scenarios are conceived, for example:

1. Brazil becomes a net exporter of natural gas to global markets.

2. The diffusion of LNG as a complementary gas supply solution for domestic markets 3. The diversification of economic agents that will find better ways to operate in more open and more competitive markets.

Preliminary results: One of the models identified and with advanced preliminary analysis refers to offshore gas production using small-scale mobile liquefaction plants, mainly in the Brazilian pre-salt areas. Due to the recent geopolitical environment, the increase in commodity prices impacts global energy markets but also generates opportunities for technological solutions that are beginning to be economically viable and whose technical and financial implementation proves to be more realistic for countries with emerging gas markets such as Brazil.

Preliminary conclusions: As preliminary conclusions, it is possible to identify concerns regarding the national natural gas market size compared to other markets in developing European countries or North American countries. As a country with vast geographical dimensions and a high population concentration in coastal cities, where the primary national industries are located, constructing a gas pipeline network to serve small populations or industries far from the centres can be costly.

Therefore, using compressed or liquefied gas modes is appropriate for transporting natural gas over long distances in small quantities. Which, in turn, will feed small-scale plants to adapt the product for use at the destination. This small-scale solution could develop the gas market in Brazil and prove a basis for developing more robust infrastructure in the long term.

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Abstract Title: New Technologies for Cars – Costs, Impacts and Advantages

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Abstract: The energy transition that is taking place in the automobile sector, characterized by the electrification of the fleet, is devoid of economic support and questionable from an environmental point of view.
Electric vehicles cost at least US$35,000.00, while conventional vehicles cost S$20,000.00 (https://afdc.energy.gov/vehicles/search/download.pdf?year=2023). The global fleet of these vehicles is in the order of one billion units and the total transformation will cost US$ 15 trillion in 20 years, or. US$ 750 billion/year, a value that is completely at odds with data from the IPCC, which predicts an annual cost of 0.1% of world GDP (US$ 80 billion) to prevent temperature increases from exceeding 2oC.
From an environmental point of view, conventional cars with an average consumption of 7.7 km/L of ethanol covering 12,500 km/year, emit 933 kg of CO2e, when we remember that the ethanol plant exports 50 kWh/L of ethanol to the electricity grid. Therefore, we have less emissions than in electric cars and with zero cost to replace the fleet. Purely electric vehicles consume 1 kWh for every 6 km of travel and thus use 2,083 kWh/year. In 2023, each kWh generated in the world emits 420 gCO2e, totalling 875 kgCO2e in annual emissions for driving a car. The manufacture of batteries and losses in electricity transmission increase this value to something close to 1000 kgCO2e.
Unfortunately, the use of electrification has already spread throughout the world, but there is still time to use it more rationally. Hybrid electric vehicles using ethanol to generate electricity in the car emit 485 gCO2e/year and cost US$27,500.00, that is an annual fleet replacement cost

of US$375 billion. Plug-in hybrid vehicles consume 359 L of ethanol and 1070 kWh, which implies an emission of 281 kg CO2e/year, remembering that the electricity comes in part from the sugar cane plant. As it costs US$32,300.00 to replace the global fleet of conventional vehicles with this one, it involves annual investments of US$615 billion. If the plug-in hybrid car is designed to operate solely on ethanol, efficiency improves to 11 km/L and ethanol consumption reduces to 279 L while electricity consumption remains unchanged – 1070 kWh when covering 12,500 km. Under these conditions, greenhouse gas emissions decline to 236 kg of CO2e per year, while the cost of replacing the fleet is the same at US$615 billion per year. Electrification brings high costs to society, but greatly increases the possibility of ethanol being accepted in a large part of the world. The amount of soil needed to produce it from sugar cane is greatly reduced. In the case of the conventional vehicle, we need 210 Mha. This value declines to 108, 46 and 36 Mha, for ethanol hybrids, plug-in flex hybrid ethanol and plug-in hybrid ethanol only, respectively.

Keywords: Electric cars, Hybrid cars, Plug-in hybrid cars, Ethanol, GHGs emissions

Introduction and Objectives: Energy transition in the automobile sector is too expensive. Other technologies are available at lower cost. Nevertheless, it is occurring and we intend to discuss technologies to minimize its huge cost imposed to society.

Methodology: Evaluation of GHGs emissions through full LCA and comparison with all costs of automobile purchase and operation for some potential technologies.

Preliminary results: The most economical alternative to conventional internal combustion automobiles is electric vehicles, followed by hybrid electric, plug-in hybrid and battery electric vehicles.The use of ethanol as the fuel guarantees low ghgs emissions in the first three options. Nevertheless, harvest area for sugar cane production will continue to be a global issue, except for the plug-in hybrid electric one.

Preliminary conclusions: Significant global acceptance of plug-in hybrid automobiles can promote the sugar cane ethanol market worldwide, and significantly contributes to climate change mitigation. Other choices may imply in ethanol global use decrease.

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Abstract Title: How much would the energy transition cost for steel and cement industries in Brazil?

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Abstract: Steel and cement are among the main challenges to solve the global climate change. Increasing the share of cleaner production routes that already exist in Brazil can reduce the fossil fuel consumption. In order to investigate CO2 reduction potential and costs related to the energy transition for these two industries, the present study developed an integrated energy transition (ET) scenario by 2050. The model is supported by a methodologic set including econometrics, Marginal Abatement Cost (MAC) analysis and Monte Carlo uncertainty method. We have found that annual CO2 emissions would exceed 250 million metric ton in the business-as-usual (BAU) scenario, and energy transition strategies can reduce 2021-2050 emissions by 52%, avoiding 2.7 billion tCO2 with an average cost of US$10/tCO2. The substitution for coal and pet coke is substantial as electricity and biocharcoal consumption increases. To achieve the maximum potential, government policies must be applied to ensure renewable energy-based electricity and sustainable timber for charcoal. The results also provide a basis for balancing the contrasting costs among ET strategies through incentives and regulatory policies, and carbon trading between steel and cement industries.

Keywords: Cost analysis, Low carbon, Carbon benchmark, Biomass, Coprocessing, Electrification.

Introduction and Objectives: Globally, steel and cement industries are responsible for 8% of the energy demand and 15% of global anthropogenic CO2 emissions. In Brazil, these industries represented 76% of industrial CO2 emissions across the last decade. Process emissions from steel and cement production increase by 15% and 54%, respectively, if energy consumption related emissions are included.

Currently, fossil fuels predominate in the energy mix of steel and cement production. Steel producers can replace mineral coal with biocharcoal in blast furnaces (BF) and electricity through electric arc furnaces (EAF). In the same way, cement producers can reduce pet coke use by increasing the share of coprocessing in the fuel mix, and introducing the refuse-derivated fuel (RDF) based on municipal solid wastes (MSW). In addition, it is possible to reduce the total thermal demand by increasing the share of supplementary cementitious materials (SCM) in the cement composition and increasing material efficiency by a market change from onsite to ready-mix concrete and mortar.

Production costs for aforementioned routes may partially explain why their representations are currently low compared to conventional routes in Brazil. In this sense, studies about future low carbon scenarios must incorporate economic analyses to engage corporative, political and social players. Economic analyses as the Marginal Abatement Cost (MAC) and break-even carbon price (BECP) are tools to estimate the amount of investments needed to implement low carbon

strategies as well as to find opportunities on economic savings, revenues and jobs generation, etc. Therefore, they can support decision-makers to stablish carbon markets, tax and/or subsidies.

Given that MAC values are broadly divergent along countries and regions, specific assessments should be carried out rather than relying on global values from literature. Moreover, although Brazil is committed with the global climate change mitigation by means of the Paris Agreement, tangible plans about low carbon pathways based on MAC are scarce. Then, the present study aimed to assess the CO2 reduction potential and costs related to the energy transition pathway for steel and cement industries in Brazil. For this purpose, we have developed an energy transition (ET) scenario, which is based on five strategies that reduce fossil fuel consumption and substitute it by renewable energy, integrating these industries until 2050.

Methodology: We developed the steel-cement integrated model through five steps, detailed next. The first step was to forecast steel and cement productions from 2021 to 2050, which was made through an econometric analysis correlating their demands with the Gross Domestic Product (GDP) per capita and Brazilian age composition. Data for 1990-2020 used to estimate multiple linear regressions came from Brazilian Steel Institute (IABr), National Union of the Cement Industry (SNIC), Brazilian Institute of Geography and Statistics (IBGE), and World Bank. Demand forecasting have been made based on the GDP forecasting used by the National Energy Plan. For cement, on the one hand, we have assumed that the demand is equal to the production for the entire period, because the relevance of international trading is low. For steel, on the other hand, we have assumed a net-export value around 9Mt/year.

The second step was the analysis on Brazilian technologic settings and the determination of a business as-usual (BAU) scenario, i.e. the maintenance of the current trend, and the ET scenario, in which energy transition strategies are implemented. To determine the penetration of strategies along the ET scenario,

we have estimated the total domestic scrap amount available for steel recycling until 2050, using an adaptation of the Scrap Availability Assessment Model (SAAM). In addition, we developed an equilibrium equation, namely break-even share (BES), to determinate the economically feasible share of biocharcoal for the BF.

The third step was to forecast emission factors for the Brazilian power generation until 2050. Based on a study on the Brazilian grid, this analysis has shown that emission factor would be 242gCO2/kWh in 2050. While this value remains lower than the global average, represents an annual increase by 3.5% from 2020 level and influences ET scenario's carbon balance.

The fourth step was the economic analysis based on MAC. MAC is the cost or saving (if it is negative) to avoid one metric ton of CO2 (US$/tCO2) and is calculated by the difference between BAU and ET scenarios in terms of emissions and costs. Cost data came from several, both national and international, sources.

The last step was an uncertainty analysis based on the Monte Carlo Method. We have randomized a set of 36 variables embracing all parts of the model according to a normal probability distribution function. We have generated 10,000 simulations and analyzed the range within 5th-95th percentiles.

Preliminary results: Model outputs have shown that steel and cement productions will increase, respectively, 4.6%p.a. and 1.7%p.a. from 2020, reaching 126Mt (±46Mt) of steel and 102Mt (±88Mt) of cement in 2050. In the median simulation, 5.2 billion tCO2 would be emitted along the entire period. Energy transition can reduce total emissions by 52% (±6%). The most promising strategy is the biocharcoal in steel BF, representing 57% (±11%) of the total mitigation. The second-best strategy is SCMs (24±6%), which reduces fossil fuel demand and sizable process emissions from clinker calcination. Total energy demand, which varies from 25EJ to 76EJ within percentiles in ET scenario, is lower than in BAU scenario within 35% of Monte Carlo simulations. Total thermal energy demand for cement production decreases by 55% due to the material efficiency (concrete and mortar industrialization) and SCM. Steel sector would become the major energy consumer, representing 93% of the total demand. Splitting by energy carrier, the most expressive reduction in the ET scenario compared to the BAU scenario is for coal coke (-85%) followed by pet coke (-65%), while biocharcoal increases by 254%. Steel increases its power demand by 117% and cement decreases by 28%, resulting in a net increasing of 94%.

Biocharcoal consumption in the ET scenario would not affect neither deforestation nor land use for food production, because it demands 23Mha (95th percentile) and the estimated national land available for the steel industry is 67Mha. However, the sensibility analysis have shown that if only 3.5% of the timber for biocharcoal production was supplied by native forest extraction, this strategy's whole potential would be impaired.

Regarding costs, the ET scenario presents a weighted average MAC equal to US$10(±20)/tCO2, with a 15% probability of economic savings (negative MAC). The ET scenario represents additional costs for the steel industry and savings for the cement industry within 94% of Monte Carlo simulations. The ET scenario would affect production costs by US$25/t steel and US$-12/t cement. From 2021 to 2050, the ET scenario demands a total investment of US$ 32.3 billion to avoid 2.7GtCO2.

Breakdown analysis shows that energy is the main cost component in the ET scenario's average MAC (49% of the NPV) and for most strategies individually. If RDF prices increase by US$1.00/GJ, coprocessing MAC increases by US$1.88/tCO2. If electricity prices increase by US$1.00/MWh, recycling MAC increases by US$0.53/tCO2 and the ET scenario's average MAC increases by US$0.22/tCO2. Finally, analysis have shown that the average MAC would decrease if, in the future, the Brazilian grid was mainly based on fossil fuel thermoelectricity. Even so, looking at the whole system, a renewable energy based grid (<60gCO2/kWh) is the better scenario for climate change mitigation as it would avoid 5GtCO2 until 2050, even it reduces fly ash availability as SCM to replace clinker and its emissions in the cement production.

Preliminary conclusions: The work's main finding is the possibility to cut by half carbon emissions from steel and cement, two of Brazilian most challenging industries on the climate change mitigation, until 2050 with an average cost of US$10/tCO2. We highlight that a groundbreaker scenario based on (e.g.) carbon capture and storage will be needed to achieve net-zero emissions, but our ET scenario is attractive because it is

based on well-known and less expensive technologies that can be implemented in short-middle run. The energy transition pathway for steel and cement will require regulatory and market mechanisms to be implemented. The research points out that the ET scenario represents different costs for each industry and the design of a carbon intensity standard and a carbon market among these industries is desirable. For example, based on the proposed ET scenario, it is possible to set a benchmark of 0.68tCO2/t steel and 0.29tCO2/t cement, from which carbon credits can be defined in a cap-and-trade system. It is essential that government holistically regulates upstream and downstream sectors in steel and cement value chains, as well as imports and exports (especially for steel). In addition, a tangible energy plan must focus on assuring renewable energy-based grid because electricity, together biocharcoal, is the main energy carry in the ET scenario (around 200TWh in 2050). Regardless it, steel producers can invest in local (e.g. wind and solar) power generation to match the high power-intensity production.
Biocharcoal demand is sizable in the ET scenario. Analysis have shown that, on the one hand, it not impair the strategy's sustainability at national level, one the other hand, regional disparities may represent social, economic and environmental challenges for biocharcoal. Regulatory and monitoring incisive policies must ensure sustainable timber for biocharcoal.
We reinforce that a joint effort by industrial and government agents, as well as civil society, will be necessary to make possible the future energy transition and a national low carbon economy.

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Abstract Title: The Crucial Role of Energy Storage Technologies in the Global Energy Transition

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Abstract: This article examines the role of advanced energy storage technologies, particularly the "electric cement" developed by Massachusetts Institute of Technology (MIT) in the global energy transition from fossil fuels to renewables. These technologies are crucial for bridging energy supply-demand gaps, reducing waste, and advancing the shift to clean energy.
Electric cement, a supercapacitor utilizing water, cement, and carbon black, offers scalable and sustainable energy storage solutions for industrial and residential use, with efficient solar energy harnessing capabilities.
Considering the geopolitical context, adopting clean energy storage systems mitigates hydrocarbon resource-related tensions and aligns with the Paris Agreement's climate goals.
This interdisciplinary study assesses the geopolitical implications of energy storage technologies, emphasizing electric cement's potential impact on global energy transition and sustainability.

Keywords: Energy Storage; Sustainable Development Goals; RCGI, Brazil; Energy Transition; Knowledge Diffusion

Introduction and Objectives: In the current global context, countries have been implementing significant incentives to promote the energy transition, moving away from the dominant era of fossil fuels to the rise of renewable energies. In 2021, at COP26, countries agreed to adopt more concrete measures to mitigate the impact of fossil fuels on the climate crisis. For this transition to be effective, it is imperative that advanced large-scale energy storage technologies are available and well-developed. Energy storage technologies are efficient n decoupling supply and demand, adjusting energy supply over time, and allowing for temporary imbalances in electricity. This characteristic enables the utilization of renewable energy surpluses, minimizing waste and increasing the share of renewable energies in overall generation. Ni-Cd batteries offer an extended lifespan and greater specific energy when compared to lead-acid batteries. Nevertheless, they come with drawbacks, including concerns about cadmium's toxicity and the memory effect that occurs when a battery begins to lose capacity due to charging cycles prior to complete discharge. In this regard, an innovative candidate technology has been developed by the Massachusetts Institute of Technology (MIT) called "electric cement." The large-scale energy storage capacity of this technology holds promising potential for industrial and residential applications. It is a supercapacitor with readily available and cost-effective resources, namely water, cement, and carbon black. These components are commonly found in nature: water is the most abundant solvent on the planet; cement is the most widely used material in construction; and carbon black is not a rare chemical element, present in various sources. When these three items are combined into a single material, the resulting cement is an excellent receiver of electromagnetic energy from the sun and an excellent conductor of electricity. From a geopolitical perspective, the implementation of clean energy storage systems plays a crucial role in the current global dynamics. This occurs in the context of the search for alternatives to hydrocarbon resources, which are becoming increasingly scarce and causing tensions between nations. Furthermore, renewable energies play a fundamental role in

achieving the objectives set in the 2015 Paris Agreement, which aims to limit the global temperature increase to no more than 1.5 degrees above pre-industrial levels. In this context, this work aims to analyse the potential of energy storage systems, with a focus on "electric cement," from a geopolitical standpoint. This is especially relevant due to the ease of obtaining these resources in the case of electric cement and its wide range of potential applications, playing an essential role in the ongoing global energy transition. In this way, we will analyse the materials of electric cement and other storage technologies.

Methodology: We will conduct a literature review, with a special focus on the pioneering study by Massachusetts Institute of Technology (MIT). In the context of an energy market predominantly based on hydrocarbons transitioning to renewable energy, the efficiency and scalability of storage systems play a crucial role. These systems allow for the decoupling of energy supply and demand, adjusting supply over time, and managing temporary imbalances in electrical supply. This flexibility is essential for optimizing the use of surplus renewable energy, such as solar, reducing waste, and expanding the share of renewable energies in the global energy mix (GALLO, et al., 2016). The MIT study focuses on the potential of supercapacitors made from widely available materials like cement, water, and carbon black for energy storage. These carbon-cement supercapacitors demonstrate remarkable energy storage capacity and high-speed charging and discharging capabilities, making them suitable for a variety of applications, from self-sustaining shelters to roads that recharge electric vehicles and intermittent energy storage for wind turbines. The research leverages the synergy between cement hydration and the use of carbon black, resulting in the formation of an electrically conductive network and hydration porosity essential for energy storage. This sustainable approach has the potential to offset the environmental impact associated with cement production, which is a significant source of CO2 emissions (CHANUT, Nicolas, et al., 2023). The work is multidisciplinary, involving geopolitics, Earth-derived resources, physics, and chemistry.

Preliminary results: In light of our initial analysis, it is clear that advanced energy storage technologies, including the innovative "electric cement," hold significant promise in driving the global energy transition forward. These technologies efficiently address the critical issues of energy supply-demand balance, waste reduction, and the promotion of renewable energy adoption. As expected, results, through this study, we intend to analyse the geopolitical viability of applying energy storage technologies, especially electric cement.

Preliminary conclusions: The potential of electric cement, utilizing easily accessible and environmentally friendly materials, cannot be overlooked. It presents a cost-effective and scalable solution for energy storage, particularly in industrial and residential contexts, thanks to its effective solar energy harnessing and electricity conduction capabilities. From a geopolitical perspective, the adoption of clean energy storage systems has the potential to alleviate tensions related to hydrocarbon resources and align with international climate objectives, as outlined in the Paris Agreement. However, it's essential to acknowledge that these

conclusions are preliminary in nature. Further, in-depth research is required to comprehensively explore the geopolitical ramifications and practical applications of energy storage technologies, including electric cement. Additional data, analysis, and real-world implementation will provide a more comprehensive understanding of their role in the ongoing global energy transition and sustainability efforts.

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Chairs: Lucy Gomes Sant Anna – Pedro Vidinha

Leonardo Domenico De Angelis
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Abstract Title: Mechanistic insights of the plasmon-enhanced CO2 reduction reaction

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Abstract: This ongoing work discusses the use of Cu2O-Au semiconductor-metal composites in the electrochemical CO2RR to produce value-added chemicals and address climate change issues. The study explores different morphologies of Cu2O materials decorated with Au nanoparticles and evaluates their electrochemical performance using various techniques, including 3D printed electrochemical cells and online Electrochemical Mass Spectrometry (EC-MS). The addition of Au appears to enhance the reduction of Cu2O in light conditions, reducing

overpotential and increasing charge transfer. The Cu2O Au materials exhibit greater selectivity for certain CO2RR products, such as CO and C2H4, over CH4. In situ FTIR Reflectance Absorption Spectroscopy (FTIR-RAS) experiments revealed that a completely different mechanism is observed in each condition, providing insights into the influence of hot carriers in the CO2RR mechanism, with light incidence breaking strongly bonded H2O molecules.

Keywords: CO2, CO2RR, carbon dioxide, electrocatalysis, electroreduction, plasmonics, LSPR.

Introduction and Objectives: High carbon dioxide (CO2) emissions are attributed as the main cause of climate change, which has far reached consequences that impact the displacement of communities and loss of biodiversity. Changing weather patterns can disrupt agriculture and lead to economic challenges. As such, one strategy to both mitigate CO2 emissions and produce value-added chemicals is the electrochemical CO2 reduction reaction (CO2RR). Cuprous oxide (Cu2O) electrocatalysts are known to be amongst the most selective for C2 chemicals (ethanol, ethylene, amongst others) production through the CO2RR. It is also possible to fine-tune the material's surface to a given preferential exposed facet and control the morphology between cubic and octahedral, as CO2RR's intermediates adsorb differently depending on the availability of active sites, partially favouring a certain mechanistic pathway.
Furthermore, the coupling of Cu2O materials with plasmonic nanoparticles, such as gold (Au), is a promising underexplored field that could boost the selectivity for C2 even further through a phenomenon called Localized Surface Plasmon Resonance (LSPR). Besides confined local heating and near-field enhancement, LSPR can be used to inject excited charge carriers ("hot electrons") generated by Au's interaction with electric fields into the conduction band of Cu2O. Au can also play a big role in generating excess carbon monoxide (CO), which can be captured and further reduced to other chemicals by the Cu2O. However, despite high efficiencies being reported in the literature, mechanistic understanding of the plasmon-enhanced CO2RR is limited, and as such, in-situ surface analysis is vital for improved molecular-level comprehension and development of optimized systems. This work synthesizes Cu2O materials of different morphologies (cubic and octahedral) decorated with Au nanospheres towards the conversion of CO2 into C2 chemicals using visible light irradiation, as well as performing online and in situ experiments to achieve mechanistic insights in the role of each variable influencing the selectivity of the CO2RR.

Methodology: Cu2O materials are synthesized in different morphologies by preparing a solution of copper chloride (II), sodium dodecyl sulphate, sodium hydroxide, and varying contents of hydroxylamine hydrochloride (HH). Higher contents of HH in the synthesis solution result in octahedra, while lower contents result in cubes. Au decoration is done by galvanic substitution of the as-prepared Cu2O materials, with the use of polyvinylpyrrolidone and chloroauric acid, resulting in a Cu2O-Au semiconductor-metal composite. The materials were characterized by several non-electrochemical techniques, such as Atomic Absorption Spectroscopy, Diffuse Reflectance and Transmission UV-Vis Spectroscopy, Fourier

Transformed Infrared (FTIR) Transmission Spectroscopy, Scanning Electron Microscopy, Transmission Electron Microscopy, and X-Ray Diffraction.
For the evaluation of the electrochemical performance of each material, custom-made 3D printed electrochemical cells were utilized depending on the application. Either a glassy carbon or carbon paper drop-casted with the Cu2O-Au materials were utilized as working electrode, a platinum (Pt) ring as auxiliary electrode and silver chloride (Ag|AgCl|KClsat) as reference electrode. The electrochemical characterization and peak reduction assignments were performed with triangular potential perturbations carried out by a bipotentiostat in a CO2-saturated potassium bicarbonate (KHCO3) 0.1 M solution. The online Electrochemical Mass Spectrometry (EC-MS) technique was utilized to follow real-time gaseous product generation (such as CO, ethylene, and methane) in the working electrode, and comparisons were made between exposed facet, presence of Au nanoparticles, and light irradiation. In situ FTIR Reflectance Absorption Spectroscopy (FTIR-RAS) was utilized for evaluating changes in the mechanism by following IR bands related to possible products and intermediates with the applied potential. Both techniques are not commonly coupled with plasmon-enhanced reactions.

Preliminary results: Electrochemical characterization of the Cu2O materials shows that Cu2O is partially reduced to Cu before the CO2RR, evidenced by a reduction peak during cathodic linear sweep voltammetry (LSV). This is corroborated by some works in literature as well. The addition of Au seems to reduce the overpotential and increase charge transfer. When illuminating the electrode, the overpotential for the Cu2O reduction is greatly reduced, which could be related to the filling of the conduction band. This effect is enhanced with the addition of Au, being an indication that Au is injecting electrons in the conduction band of the Cu2O and therefore more easily allowing electron transfers. During online EC-MS, results show that CH4 is greatly mitigated with the addition of Au, and the more favourable pathway shifts for the formation of CO, while C2H4 production is roughly similar. The synergy between Cu2O and Au was more pronounced while utilizing the cubic materials. This is in agreement with reported works that exhibit a preference for CO and C2H4 over CH4 production when the preferential exposed facet of the catalyst is 100 instead of 111. When illuminating the electrode, a decrease in production of CH4 is observed, while all other gaseous products have their generation increased. As such, plasmon enhancement might be related to a release of *CO intermediates instead of hydrogenation. This was observed in similar works which argue that local heating might be favouring CO desorption, which in turn increases availability of active sites and increases electrochemical current. Our work suggests that the employment of both Au and light irradiation broadens the potential range in which little to no CH4 production is observed, which can be interpreted as higher selectivity for certain products amongst the several possible products of the CO2RR.
More recently, our group has begun tests with plasmon-enhanced FTIR-RAS experiments. Very few works have attempted to elucidate the hot-carrier influence in the CO2RR mechanism. Preliminary results showed that the behaviour of interfacial H2O molecules is completely different in each condition for the cubic materials (“Cu2O/dark”, “Cu2O-Au/dark”, “Cu2O-

Au/light"), and a proper evaluation of each situation is still undergoing. In the "Cu2O/dark" condition, lower overpotentials result in negative absorbance of O-H stretching and H-O-H bending bands, suggesting H2O consumption, possibly related to CO2 adsorption and HCOOH generation. Similarly, the "Cu2O-Au/dark" condition shows similar behavior but with pronounced H bonding and C2 production indicators. In the "Cu2O-Au/light" condition, light exposure sharpens the signal for "ice-like" H2O, indicating the breakage of stronger H-bonds. Corroboratively, higher positive signals and increased interfacial pH suggest proton consumption and OH- formation, as observed through the CO32- adsorption band.

Preliminary conclusions: The electrochemical characterization of Cu2O materials, particularly in combination with Au, revealed significant insights into their behaviour during the CO2RR. The addition of Au appeared to enhance charge transfer and reduce overpotential, with even more pronounced effects observed when illuminated. This suggests that Au may inject electrons into the conduction band of Cu2O, facilitating electron transfers. Online EC-MS results indicated that the presence of Au mitigated CH4 production, favouring the formation of CO, especially in the case of cubic materials. The synergy between Cu2O and Au in promoting CO and C2H4 production over CH4 aligns with previous studies. Furthermore, plasmon enhancement, potentially related to the release of *CO intermediates, may contribute to this selectivity by favouring CO desorption and increasing active site availability. Additionally, preliminary plasmon enhanced FTIR-RAS experiments highlighted the distinct behaviour of interfacial H2O molecules, shedding light on potential pathways for CO2RR intermediates like HCOOH generation. Overall, these findings provide valuable insights into the mechanisms of the CO2RR, offering avenues for enhancing selectivity and efficiency in producing valuable chemicals from CO2. Further investigations are warranted to fully understand the hot-carrier influence and optimize these materials for practical applications.

Lorenzo Kęsikowski Follador
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Abstract Title: Screening of Ionic Liquids for CO2RR using Molecular Dynamics
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Abstract: We used Molecular Dynamics to perform a screening of 18 Ionic Liquids of electrochemical importance. All of the ionic liquids were based on 6 phosphonium cations, which prevent parasite reactions from occurring, thus enhancing faradaic efficiency of the whole process. The 3 anions considered are of proven electrochemical capacity. The ILs ability to solubilize CO2 was evaluated using computational methods. Two of the best ionic liquids

were selected for further studies, which included structural characterization and transport properties evaluation. We found that there is no significant difference between.

Keywords: CO2 reduction, Molecular Dynamics, Ionic Liquids.

Introduction and Objectives: We urgently need new carbon capture, storage, and utilization (CCSU) methods to limit Earth's temperature rise to 1.5ºC (IPCC AR6 WGIII Technical Summary). Current technologies use energy intensive, corrosive amine-derived solvents degraded by NO2, SO2, and O2 (Leung 2014; Aghaie 2018). Ionic liquids (ILs) are proposed alternatives due to stability, low vapor pressures, and environmental benefits (Aghaie 2018). Some ILs absorb CO2 chemically (Almantariotis 2012; Li 2021), but energy costs for gas release limit their utility. Efficient carbon reduction reactions (CO2RR) require a wide electrochemical window, transport properties, and gas dissolution (Wang 2020; Monteiro 2011). Phosphonium ions (P_XXXY^+) are proposed cations due to stability and absence of acidic hydrogens, overcoming overpotential issues (Martins 2015; SnchezRamrez 2017). Their carbon side-chains can be adjusted for improved properties (Khalil 2020). Combining phosphoniums with effective anions creates diverse ILs for CO2RR. We used Molecular Dynamics to screen 18 ILs, identifying [P1444][FSI] and [P1444][TFSI] as promising for further analysis (Martins 2015). Further evaluation involved interaction energies, Henry Constants, structural analysis, and transport properties. Notably, [P1444][TFSI] exhibited promising characteristics in line with computational predictions.

Methodology: We used both computational and experimental methods to determine the suitability of a family of ionic liquids for CO2RR. Molecular Dynamics were used to screen 18 ionic liquids based on their ability to solubilize CO2. The gas solubility was determined using free-energy and Henry constant calculations. The best suited ionic liquids were then selected for further computational analysis, which included structural characterization (evaluated by radial and spatial distribution functions), thermodynamic parameters (with enthalpy and entropy determination) and interaction energies (Lennard-Jones and Coulomb). One of the ionic liquids was then subjected to viscosity and density measurements of pure and CO2-saturated solution. The absolute solubilization capacity of this IL was determined by magnetic suspension balance.

Preliminary results: Of the 18 ionic liquids, those made of P1444+ cation presented the best options for CO2 solubility, as their henry constants returned lower on computational evaluation. Furthermore, the entropy and enthalpy of dissolution does not seem to vary much, which suggest that interspecies interactions are responsible for the higher solubility of CO2 in [P1444][TFSI] than on [P1444][FSI]. Indeed, structural characterization showed a significant role of fluorines in interacting with CO2, which explains the previous results. Experimental measurements then confirmed the decreased density and viscosity of IL when CO2 is dissolved, but, as in the simulations, the variation was limited and did not improve transport properties significantly.

Preliminary conclusions: In this work, we have screened 18 possible ionic liquids (ILs) for the CO2RR. We found that the P1444+ series has the best solubility of CO2. Thermodynamic calculations showed that the dissolution of carbon dioxide in [P1444][TFSI] is less sensitive to temperature variations than in [P1444][FSI]. The radial distribution functions of CO2 in both ILs showed that the gas molecule is similarly distributed around the ions. The mobility of cations and anions for the P1444+ series was evaluated for each calculated concentration of carbon dioxide. As expected, every species displayed higher mobility when more gas had been dissolved. The calculated study was confronted with the measured density, viscosity, and CO2-

solubility for the available [P1444][TFSI]. It was found that the real systems followed the expectations of the simulations. However, the solubility results from the MSB were even lower than the lowest calculated concentration. This suggests that any following studies regarding carbon dioxide in ILs may need to reassess the presented thermodynamic evidence.

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Abstract Title: Utilizing Microalgae for Sustainable Biorefinery: A Path to Carbon Mitigation and Bioeconomic Prosperity

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Abstract: Population growth and industrialization have generated serious pollution issues due to uncontrolled emissions of greenhouse gases and industrial effluents. Climate change has

underscored the importance of reducing CO2 emissions and finding ways to sequester them. The UN has launched the 2030 agenda with 17 sustainable development goals, aiming for renewable resources and a sustainable production and consumption system. Microalgal photosynthesis offers energy solutions, food security, and climate change mitigation by absorbing 10 times more CO2 than terrestrial plants. Microalgae are unique microscopic cells that can be either prokaryotic (cyanobacteria) or eukaryotic, such as green microalgae, and they have wide adaptability to different environments. They produce valuable biomolecules and are considered "cell factories" and candidates for CO2 mitigation. Microalgae have several advantages: rapid growth, adaptability to extreme environments, and an environmentally friendly ecological profile. Integrating microalgae into a biorefinery can promote a circular bioeconomy, where CO2 is mitigated and products are obtained. This work aimed to achieve desired levels of biomass productivity using 5% CO2 and obtain bioproducts such as carbohydrates and lipids for potential biofuel production, pigments, and proteins with potential nutraceutical and pharmaceutical uses. The strain studied in this project was identified as Dictyosphaerium sp. The cultivation was carried out in two stages, with the first stage using complete BG11 medium to obtain biomass and the subsequent stage using nitrogen-free BG medium (BG-Nfree) to accumulate bioproducts. Growth was conducted over 168 hours with a final volume of 400 mL, 5% CO2 bubbling, and a 24-hour photoperiod with a light intensity of 10,000 Lux. The biomass obtained during the growth phase was 1 g/L, and its weight doubled after the bioproduct accumulation period. After 168 hours of growth, the culture was centrifuged to change to BG-Nfree medium. The accumulation phase lasted for 11 days. For carbohydrate production, the best result was achieved in 7 days with a carbohydrate yield of 43% (with 39% being glucose). The other products analyzed included lipids with 27% (±3.5) proteins, and pigments 298 µg/mg (±18.57). The results demonstrate the potential of the Dictyosphaerium sp. strain for use in the biorefinery concept, particularly to produce third-generation ethanol, owing to its high carbohydrate production.

Keywords: biorefinery, CO2 mitigation, microalgae, bioproducts.

Introduction and Objectives: Population growth and industrialization have generated serious pollution issues due to uncontrolled emissions of greenhouse gases and industrial effluents. Climate change has underscored the importance of reducing CO2 emissions and finding ways to sequester them. The UN has launched the 2030 agenda with 17 sustainable development goals, aiming for renewable resources and a sustainable production and consumption system. Microalgal photosynthesis offers energy solutions, food security, and climate change mitigation by absorbing 10 times more CO2 than terrestrial plants. Microalgae are unique microscopic cells that can be either prokaryotic (cyanobacteria) or eukaryotic, such as green microalgae, and they have wide adaptability to different environments. They produce valuable biomolecules and are considered "cell factories" and candidates for CO2 mitigation. Microalgae have several advantages: rapid growth, adaptability to extreme environments, and an environmentally friendly ecological profile. Integrating microalgae into a biorefinery can promote a circular bioeconomy, where CO2 is mitigated and products are obtained. This work aimed to achieve

desired levels of biomass productivity using 5% CO2 and obtain bioproducts such as carbohydrates and lipids for potential biofuel production, pigments, and proteins with potential nutraceutical and pharmaceutical uses.

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Preliminary conclusions: The results demonstrate the potential of the Dictyosphaerium sp. strain for use in the biorefinery concept, particularly to produce third-generation ethanol, owing to its high carbohydrate production.

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Abstract Title: Effect of the catalyst copper loading on the ethanol production in the CO2 hydrogenation over Cu-UiO-67

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Abstract: The hydrogenation of CO2 to products of commercial interest, such as alcohols, can reduce the dependence on fossil resources. However, in this reaction, CO2 conversion, products selectivity and catalyst stability are challenges to be overcome. In this context, metalorganic-frameworks (MOFs) are interesting materials to be applied as catalyst support in the CO2 hydrogenation, as they can generate stable interfaces with active sites, protecting them from deactivation. Furthermore, with MOF-supported catalysts the control of specific sites is possible, making them more selective for the product of interest. Therefore, they can be useful to improve the production of alcohols, such as ethanol. Knowing that, this work aims to synthesize Cu-UiO-67 and apply it in the CO2 hydrogenation under mild conditions to produce

ethanol. UiO-67, which is a specific MOF, used in the present work as a support for Cu active sites, was synthesized by solvothermal method for 48 h at 120°C. Nominal copper lading of 10-60 wt.% was incorporated into its structure via ion exchange. The CO2 hydrogenation was carried out at atmospheric pressure, during 3h, 260 °C and under H2/CO2 molar ratio of 3/1. Reaction products were identified and quantified via GC-FID and GC-TCD. Using XRD, SEM, FTIR and H2-TPR, it was possible to investigate, respectively, the formation of crystalline structures, morphology, the presence of functional groups, and the reducibility of the catalyst. The effect of copper loading on the CO2 hydrogenation reaction was explored. preliminary results showed that ethanol, methanol, CO and acetaldehyde have been produced. The most promising ethanol production was observed when Cu-UiO-10 (with 10 wt% Cu) was used as catalyst, while the highest methanol productivity, 633 µmolMetOH/h.gcu, occurred on Cu UiO-20 (with 20 wt.% Cu). The selectivity of CO reached a maximum of 20% (Cu-UiO-30). On the other hand, the selectivity of alcohols decreased with increasing copper loading, but remained above 70% for both alcohols.

Keywords: CO2 hydrogenation, UiO-67, copper loading.

Introduction and Objectives: The possibility of capturing and transforming CO2 into products of commercial interest, such as alcohols, via hydrogenation, linked to the use of renewable energy, can curb the indiscriminate emissions of this gas and reduce dependence on fossil resources. On the other hand, the CO2 hydrogenation reaction presents some challenges, such as increase the conversion of CO2 at mild conditions, as well as the selectivity to the product of interest (in this case ethanol), avoid the deactivation of active sites under reaction conditions, and use clean hydrogen generated by renewable sources. In this context, metal-organic frameworks (MOFs) seem interesting to be used as support of catalysts applied to this reaction, as they have the characteristics of generating stable interfaces with active sites, for example by confining them in their secondary building units (SBUs). Zirconium-based MOFS (Zr-MOFs), more specifically, have a surface rich in oxo groups and hydroxides, which favor the interaction between the support (MOF) and the active site, being beneficial to the catalyst stability and activity. Furthermore, MOFs allows us to control specific sites of the catalyst, making it more efficient for the product of interest. In this way, it can be useful for improving the synthesis of higher alcohols, such as ethanol. Knowing this, the present work aims to explore MOFs as support for copper active sites and study the catalytic performance of these materials in the CO2 hydrogenation at atmospheric pressure. The effect of catalyst copper loading on the production of alcohols, mainly ethanol, was evaluated.

Methodology: The synthesis of UiO-67 was carried out via a solvothermal method. In a typical experiment, zirconium (IV) chloride (ZrCl4, 0.6292 g), the organic linker 4,4-biphenyldicarboxylic acid (H2bpdc, 0.6540 g), dimethylformamide (DMF, 150 mL) and formic acid (HCO2H, 14.71 mL) were added to a flask with a capacity of 250 mL. This mixture was kept in ultrasound until all solids dissolved. The homogenized solution was placed in an oven at 120 °C for 48 h to produce the UiO-67 structure. Then, the material was separated by

centrifugation (10000 rpm, 10 min) and washed sequentially with DMF (15 mL), tetrahydrofuran (THF, 15 mL) and acetone (15 mL) 3 times for 24 hours. The resulting solid was dried in an oven at 60 °C for 24 h. The synthesis of the material resulted in a yield close to 60%. The addition of copper to the UiO-67 structure was carried out via ion exchange. Initially, UiO-67 (0.6 g) was added to an aqueous solution of copper acetate (AcCu). The nominal copper loading (10-60 wt% Cu) was controlled by using distinct concentrations of AcCu aqueous solution. The suspension was kept under stirring (500 rpm) at room temperature for 24 h. It was then placed in three vials, and the material was separated by centrifugation and washed, also for 24 h. Deionized water and acetone were used for washing. First, 30 mL of deionized water were added to the solid contained in each bottle and then the mixture was centrifuged. This cycle was repeated three times. Then, 30 mL of acetone were added to each one of the vials, kept in contact with the solid for 8 hours, and then the material was centrifuged. This procedure was also repeated three times. Finally, the washed solid was dried in an oven at 60 °C for 12 h. The resulting materials were characterized by X-ray diffraction (XRD) to investigate the crystalline structure of the as-synthesized and Cu-containing UiO-67. Scanning electron microscopy (SEM) was employed to explore the morphology of the as-synthesized UiO-67, temperature programmed reduction with H2 (H2- TPR) was carried out to study the reduction behaviour of the catalyst copper species and the Fourier transform infrared spectroscopy (FTIR) technique was used to investigate the characteristic bands of the functional groups present in the as-synthesized UiO-67, as well as to evaluate the maintenance of these bands after the metalation step. CO2 hydrogenation was performed at atmospheric pressure. Before the reaction, the catalyst was activated under H2 stream at 280 °C for 1h. Then, the reaction was carried for 3 h at 260 °C, using a H2/CO2 molar ratio of 3/1. Products were quantified via GC-FID and GC-TCD.

Preliminary results: *By analysing the XRD profiles, it was possible to observe peaks at 5.62°, 6.46° and 9.18°, which are assigned to the (111), (002) and (022) diffraction planes of UiO-67. After the copper incorporation on the support, the material crystallinity reduced and this effect was intensified with increasing nominal copper loading. The SEM images revealed that the support contains particles with well-defined faces and edges, in addition to a smooth surface with a regular octahedral crystal shape. This shape remained stable after the copper addition. Infrared spectra show the characteristic vibrational bands of UiO-67 functional groups, including the presence of the collective vibrational modes of the organic linker used in the synthesis of the MOF, vbpdc. These bands were also observed for the Cu-containing material. By H2-TPR, it was possible to observe two overlapping peaks with different intensities associated with the direct reduction of Cu2+ to metallic copper. Tactivation was chosen based on the thermal stability of these materials (ca. 300 °C) and RTP-H2 results, which show that the complete reduction of the investigated catalysts occurs at temperatures close to 280 °C. At the studied conditions, it was possible to verify the formation of alcohols, acetaldehyde, and CO as reaction products. Increasing the nominal copper loading from 10 to 30 wt.% resulted in a positive impact on the methanol productivity and an increase in CO selectivity. On the other hand, the catalyst containing 10% wt. of Cu presented the best performance for the formation

of ethanol, reaching a productivity of 57.2 µmolEtOH h-1 gCu-1. Increasing the Cu loading up to 60 wt% (UiO-Cu-60) led to a drastic drop in the ethanol productivity. Additional studies are in progress, aiming to further characterize the materials and understand their catalytic performances.

Preliminary conclusions: The influence of copper loading on the production of alcohols in the CO2 hydrogenation over Cu-UiO-67 at ambient pressure was investigated. Ethanol productivity reached a maximum of 57.2 µmolEtOH h-1 gCu-1 on the UiO-Cu-10. In addition to alcohols, CO and acetaldehyde have been produced. Complementary analyses of the catalysts with different copper loadings are in progress.

Lucas Rodrigues da Silva
IQ - USP

Abstract Title: Synthesis and Characterization of CuFeZn-based Materials as Catalysts for CO2 Hydrogenation

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Abstract: In this study, we explored the synthesis and catalytic properties of Cu1FexZn1 catalysts, where the parameter x varied from 0 to 1.5 in increments of 0.5. The primary focus of our investigation was the impact of iron (Fe) addition on the selectivity profile during the hydrogenation of carbon dioxide (CO2). Our findings revealed significant changes in product selectivity with the introduction of Fe into the system. In the absence of iron (x=0), the CuZn catalyst primarily produced methanol. However, when iron was introduced at x=0.5, the selectivity shifted towards methane. Furthermore, an increase in iron concentration (x=1.0 and 1.5) led to a predominant production of long-chain hydrocarbons (C5+), accompanied by an increase in CO2 conversion, while the selectivity for carbon monoxide (CO) remained relatively consistent. These results demonstrate the tunable catalytic properties of Cu1FexZn1 catalysts in CO2 hydrogenation, offering insights into their potential for the selective synthesis of various valuable products, such as long-chain hydrocarbons.

Keywords: CuFeZn, CO2, Catalyst.

Introduction and Objectives: The escalation in CO2 emissions is primarily attributed to the ongoing dependence on fossil fuel derivatives to satisfy energy demands [1]. Consequently, it has become imperative to implement strategies for mitigating emissions, with one notable approach being carbon capture and utilization (CCU). In this framework, the conversion of CO2 into valuable products presents a promising avenue for addressing this environmental concern.

Among various systems, the CuFeZn catalyst has emerged as a highly effective catalyst for the conversion of CO2 into ethanol [2]. Nevertheless, the existing methodology for synthesizing these catalysts typically involves coprecipitating metallic oxides followed by a calcination process. In our work, we leveraged our expertise to fabricate CuFeZn nanoparticles supported on N-doped carbon material [5] using the molten salt method. This material exhibited exceptional catalytic potential for the hydrogenation of CO2 into hydrocarbons.

Methodology: For the synthesis of catalysts, a mixture comprising acetate salts of metallic precursors (Cu, Fe, Zn), urea, and gallic acid was prepared. This mixture was subsequently subjected to pyrolysis under an inert atmosphere at a temperature of 500ºC for a duration of 4 hours. The resulting catalysts underwent comprehensive characterization through various analytical techniques, including H2 temperature programmed reduction (H2 TPR), O2 temperature-programmed oxidation (O2 TPO), X-ray diffraction (XRD), and CO2 temperature-programmed desorption (CO2 desorption). Catalytic assessments were conducted within a fixed-bed hastelloy steel reactor, with operating pressures of 20 bar, using a gaseous feed mixture consisting of 25 vol % CO2 and 75 vol % H2, delivered at a total flow rate of 20 mL/min. Prior to the commencement of the catalytic reactions, the catalysts were pre-reduced at a temperature of 500°C under a continuous flow of hydrogen (H2) for a duration of 1 hour. Subsequent to the reactions, the generated products were subjected to analysis using an Agilent gas chromatography/mass spectrometry (GC/MS) instrument, which was equipped with thermal conductivity and flame ionization detectors. Gas-phase products were analysed in situ using GC/MS, while liquid-phase products were condensed at a temperature of 15°C and subsequently analysed upon completion of the reaction.

Preliminary results: In this study, we synthesized various catalysts denoted as Cu1FexZn1, where the parameter x ranged from 0 to 1.5 in increments of 0.5. Our catalytic assessments revealed that the introduction of iron (Fe) into the system had a substantial impact on the selectivity profile during CO2 hydrogenation. Notably, when no iron was present (x=0), the CuZn system primarily produced methanol as the main product. However, with the introduction of iron at x=0.5, the selectivity shifted towards methane as the predominant product. Furthermore, an increase in iron concentration at x=1.0 and 1.5 resulted in a significant shift towards the production of long-chain hydrocarbons (C5+), becoming the major products. Interestingly, the conversion of CO2 increased with the addition of iron, while the selectivity for carbon monoxide (CO) remained relatively constant.

Preliminary conclusions: These results demonstrate the tunable catalytic properties of Cu1FexZn1 catalysts in CO2 hydrogenation, offering insights into their potential for the selective synthesis of various valuable products, including long-chain hydrocarbons, depending on the iron concentration.

Maitê Lippel Gothe
IQ-USP

Abstract Title: Scale up of a ReOx/TiO2 catalyst for the CO2 hydrogenation to methanol

Authors' Names & Affiliation Institutions of all authors (in order for publication): Institute of Chemistry, University of Sao Paulo (all authors)

Abstract: This project aims to produce pelletized ReOx/TiO2 catalysts used in a scale up project of a high-pressure flow process of CO2 hydrogenation to CH3OH. A crucial part of this project is the development of structured catalyst pellets which will withstand the harsh conditions of a high-pressure reactor while still maintaining the active and selective properties presented in the powdered catalyst.

Keywords: Scale up, Methanol, Catalysis.

Introduction and Objectives: Reducing air pollution and combating climate change caused by greenhouse gas emissions by converting them into relevant chemicals presents an intriguing path to explore within the realm of green chemistry. One potential strategy involves the conversion of CO2 into valuable chemicals, such as methanol, which is considered one of the most promising platform molecules directly obtained from CO2. To ensure a selective and efficient process, it is desirable to operate at high pressure and low temperature due to thermodynamic considerations. Additionally, the choice of catalyst significantly influences the activity and selectivity of the reaction. Re catalysts have been the subject of frequent study in hydrogenating carbonyl and carboxyl groups, showing strong selectivity toward the hydroxyl group. Recently, the author of this project reported a high pressure, supercritical flow process for converting CO2 to CH3OH using a Re catalyst, achieving 98% selectivity for CH3OH with an 18% conversion of CO2 at 100 bar and 200 °C. Furthermore, it was observed that ReOx/TiO2 exhibits superior selectivity and activity compared to other supports and metals (e.g., Ir, Pt) supported on TiO2. Based on the success of this laboratory-scale reaction process, funding was secured for scale up project aimed at producing methanol from CO2. During the scale-up process, it is necessary to modify the particle size and shape of catalysts to prevent heat and mass transfer limitations, hot spots, and excessive pressure drop in the catalytic bed, thus minimizing fouling of the catalytic phase. One way to approach the production of pelletized catalysts is to impregnate rhenium species onto commercially available pellets, although that presents challenges of its own. These are the preliminary results that will be discussed here.

Methodology: The catalysts of general composition ReOx/TiO2 are synthesized either by wet impregnation of TiO2 pellets with a ReO4- aqueous solution or by making pellets from a powder form of TiO2 already impregnated with rhenium. The soluble rhenium species ReO4- can be generated either from Re2O7 or from NH4ReO4. These catalysts are then calcined at

various temperatures ranging from 200 to 400 °C and reduced with H2 in temperatures ranging from 250 to 500 °C. The catalytic materials are then characterized with regard to their crystalline structures, surface properties, and reactivity in the CO2 hydrogenation reaction.

Preliminary results: The pelletized catalysts have shown interesting activity in the reaction, although their selectivity is not the same as the powdered form catalyst. An attempt is made to relate this to the chemical composition of the materials.

Preliminary conclusions: There are many advantages to pelletized catalysts, as well as many challenges to produce them. While our laboratory-scale process for converting CO2 into methanol using Re catalysts shows promise, optimizing pelletized catalysts is essential for scale up projects. However, additives and processes used for pelletization impact the catalytic properties of the material.

Primaggio Silva Mantovi
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Abstract Title: Controlling the Role of Water with Ionic Liquids in CO2RR Aiming C2+ Products

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Abstract: This study explores the use of Ionic Liquids (IL), specifically P1444TFSI, with controlled water content as a novel solvent system for electrochemical carbon dioxide reduction reactions (CO2RR). Unlike traditional acetonitrile (ACN) as solvent, as well as KHNO3, this approach aims to use very small amounts of electrolyte (~3 mL) to enable the use of pure IL. Copper Oxide serves as a catalyst, demonstrating its potential for producing not only metanol and acetone, an alcohol and a C3 product, but also butane, a C4 product. Gas Chromatography coupled with Mass Spectrometry (GC-MS) and Nuclear Magnetic Resonance spectroscopy (NMR-H and C) are employed for product detection and quantification. This project combines the unique properties of IL, controlled water content, copper oxide catalysts, and precise analytical tools to advance the understanding of CO2RR, leading to advances for enhancing the selective CO2 reduction, avoiding parallel reactions as Hydrogen Evolution Reaction (HER).

Keywords: Ionic Liquids, CO2RR, Electrocatalysis, C2+ Products.

Introduction and Objectives: With emerging technologies for Greenhouse Gas (GHG) transformation, the utilization of Ionic Liquids (IL) has emerged as a pivotal strategy. With the increase in these gases, particularly carbon dioxide (CO2), it has become crucial to develop efficient methods for their eco-friendly transformation into valuable fuels and chemicals. Carbon capture and utilization (CCU) represents a proactive approach to addressing this challenge. Leveraging the unique properties of IL as electrolyte and C2+ product enhancer for the Carbon Dioxide Reduction Reaction (CO2RR), this project aims to facilitate the effective conversion of CO2. This can lead to advances in the scientific community's understanding and application of these technologies, paving the way for a sustainable future where greenhouse gases are not just captured but also transformed into valuable resources for the benefit of society and the environment using renewable sources coupled with electrocatalysis. In a nutshell, the objective of this work is to understand the influence of water and its quantity on CO2RR. Coupled with a copper oxide catalyst, it aims to selectively promote alcohols and C2+ products while avoiding parallel reactions, such as the hydrogen reduction reaction (HER).

Methodology: For the electrolyte preparation: Previously dried P1444TFSI at 60°C in a glovebox with an argon atmosphere was sealed in a glass vial, and a controlled amount of water was added. Karl Fischer was used to verify the actual amount of solubilized water. For the electrode preparation: A 97% purity copper foil was used as the substrate for copper oxide electrodeposition. The electrochemical cell consisted of copper, carbon paper, and Ag/AgCl with Cl saturation as the working, counter, and reference electrodes (WE, CE, and RE), respectively. The electrolyte was CuSO4 0.3 M at pH 12 at 60°C. A chrono-potentiometry was conducted for 2 hours with 50 uA cm-2. For the electrolysis: A homemade 3D cell was used with copper oxide, platinum, and silver as the WE, CE, and pseudo-RE, respectively. A glass microfiber was used to separate the WE from the CE to avoid reoxidation of reduced products. A cyclic voltammetry was performed to evaluate the WE profile before the chrono-amperometry at -0.25 V vs Ag.

Preliminary results: The profiles of the voltammetry experiments have shown that carbon dioxide (CO2) can be only selectively reduced In the presence of water. This mean that water has a significant role in CO2 reduction reaction. The current peak only appears when water is present, demonstrating its meaningful role. Using gas chromatography-mass spectrometry (GC-MS) in parallel with nuclear magnetic resonance for hydrogen and carbon (NMR-H and C), it was possible to detect the production of methanol, acetone, butane, and other products.

Preliminary conclusions: Ionic Liquids (ILs), more specifically P1444TFSI, are able to facilitate the selective carbon dioxide reduction reaction (CO2RR) with significantly low overpotential and a wide electrochemical stability window (ESW). With this type of electrolyte, water is crucial for enabling this reaction because of the necessity of protons in the environment, and by controlling its amount, parallel reactions such as the hydrogen evolution reaction (HER) can be managed and even avoided, depending on how negative the potential is. The results not only prove that ILs are extremely useful for enabling the C-C coupling between intermediary

species at the surface of the electrode but also demonstrate the successful formation of C4 products, such as butane, a very difficult molecule to synthesize by CO2RR.

Renato Vitalino Gonçalves
University of Sao Paulo

Abstract Title: Green Hydrogen Production via Photo(electro)catalysis: BiVO4 as case of study

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Abstract: Photoelectrochemical (PEC) water splitting has been considered as a promising technique for converting solar energy into clean and renewable hydrogen (H2) fuel. Recently, bismuth vanadate (BiVO4) has attracted attention for generating green H2 solely through water and solar energy. In this study, we synthesized BiVO4/FeNiOx photoanodes using magnetron sputtering deposition. These materials were integrated into a straightforward and cost-efficient Tandem PEC cell to facilitate oxygen and hydrogen evolution reactions (OER and HER), respectively. Notably, the BiVO4/FeNiOx photoanode
displayed remarkable PEC performance and demonstrated robust chemical stability in OER, achieving a high photocurrent density of +1.22 mA cm-2 and an impressive charge transfer efficiency of 96% at the water oxidation potential. Additionally, we introduced a practical model based on classical band theory to assess the interfacial band alignment of photoelectrodes during PEC water splitting under operational conditions. Encouragingly, our novel BiVO4/FeNiOx device efficiently produced green hydrogen through a simple and robust process, maintaining stable operation for at least 5 hours.

Keywords: Water Splitting, Green hydrogen, renewable energy

Introduction and Objectives: Photoelectrochemical (PEC) water splitting has been considered as a promising technique for converting solar energy into clean and renewable hydrogen (H2) fuel. In this study, we synthesized BiVO4 photoanodes using magnetron sputtering deposition. These materials were integrated into a straightforward and cost-efficient Tandem PEC cell to facilitate oxygen and hydrogen evolution reactions (OER and HER), respectively. The primary aim of this study is to investigate the deposition of BiVO4 films with an appropriate electronic configuration for enabling green hydrogen production through PEC water splitting.

Methodology: All materials were synthesized using the magnetron sputtering deposition technique. Bismuth vanadate (BiVO4) films were deposited onto a conductive glass substrate at different times to achieve an optimal thickness, ensuring efficient light absorption and

promoting effective charge transfer at the surface, thus facilitating the water splitting reaction. The photocatalytic experiments were conducted in a hermetically sealed reactor, employing a KBi-based electrolyte with a pH of 9.3. For simulating solar irradiation, a solar simulator equipped with an AM1.5G filter, calibrated to provide an irradiance of 100 mW/cm², was employed as the light source.

Preliminary results: XRD, XPS, UV-Vis, SEM, green hydrogen production.

Preliminary conclusions: Our novel BiVO4/FeNiOx device efficiently produced green hydrogen through a simple and robust process, maintaining stable operation for at least 5 hours.

0911 – SRS19 (TV3)

Chairs: Edmilson M. dos Santos – Karen Mascarenhas

Dindara Silva Galvão
University of Sao Paulo

Abstract Title: Future literacy towards climate changes using theatre of the oppressed

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Abstract: This project aims to increase scientific dissemination and improve the public perception of science using ArtScience intersections. These explorations aim to develop and apply creative processes with active artistic experimentation workshops with the public for scientific communication centred on environmental education in non-formal spaces. It uses performing arts, particularly the theatre of the oppressed, as a methodology to improve Future Literacy. Raising attention, fomenting actions, and encouraging novelty thinking about the planet's future. This project is part of a larger project (Project 70) from the Research Center for Greenhouse Gas Innovation (RCGI). It is also part of the USP Sci-art Digital lab actions at the Institute of Physics of the University of São Paulo. It is a creative space created to promote the interdisciplinarity of science, arts, and innovation.

Keywords: ArtScience; future literacy; climate change; environment; non-formal educational spaces; performing arts.

Introduction and Objectives: The planet is now in the Anthropocene Era, i.e., an era in which

human actions have drastically modified the environment and are now dealing with the consequences of this unrestrained exploitation of natural resources. We must change how we inhabit and relate to the earth to reduce the devastation already caused and minimise its adverse effects on the planet. New technologies, legislation, and, most importantly, new ideas are essential to construct a liveable future for humanity and prevent the fast extinction of all species. However, the processes to solve all of these climate damages involve complex thinking and the active involvement of society. Besides the difficulty of public engagement in such a subject, another challenge resides in the lack of an important skill: the ability to imagine futures. Our mental capacity, as humans, only extends to thinking about the immediate or medium-term consequences of our actions. Every small step can have a significant impact not only in the present moment or the near future but also in the long term. Humanity's choices now influence the legacy we leave for the next generations and even in our future as a species, catalysing or delaying the process of evolution or extinction. To improve this skill, UNESCO coined the term Future Literacy. It is a concept that analyses and systemises how our brains unconsciously predict and plan the future, casting light on these processes. Learning these mechanisms allows the future literate person to use this brain algorithm to predict the future more actively, bringing engagement and awareness of the importance and consequences of each individual or community action. The project uses an assertive communication and engagement language: the performing arts to assist future literacy. In particular, a specific methodology was created by a Brazilian practitioner, drama theorist, and political activist called Theatre of the Oppressed. Such methodology centres on the belief that all theatrical practices are necessarily political, and one of the most fundamental principles of the technique is the withdrawal of the passive position of the spectator to dislocate them to a part of the spect-actor, i.e., leaving the comfortable place of external witness, to a more active one, in which they participate directly in the play, game or scenic experience. The theatre of the oppressed was made to be experienced by anyone, actors or non-actors. Other important pillars of Boal's technique are the collective experience of the proposed games, but always taking into consideration the subjectivity and the contexts of each of the spect-actors, revealing dynamics of oppression that they are imposed, and by doing so, transforming the individual and by extension the environment in which they are inserted.

Methodology: Through the intersection between the concepts presented: climate change, future literacy, and theatre of the oppressed, the project aims to find effective dynamics to address the theme through experimentation of creative processes along with scientific communication, emerge new discussions, comprehensions, intuitions, and ideas to build better horizons for the course of humanity. The project is structured in the steps below:
Act 1 (Conception)— Election of the ArtScience fields of exploration, mapping what has already been published in each direction and if any production combines any of them. Researching, consulting professionals in each area, using collected data from social physics in social media, etc.
Act 2 (Exploration and Experimentation) – Introduction of the performing arts involved, scientific documentation of the topics that will be addressed regarding the environment, and relating both to the theory of Future Literacy. Start to test interventions, understanding what

emerges in each practice and how the peculiarities of each group play a role in the development of the practice, as well as seeking possible similarities to systematise. Act 3 (Realization and dissemination) – Curating the games and dynamics that compose the workshop, execution of it in different and similar spaces, and collecting previous and subsequent data through surveys to analyse how the interventions influenced the perception and conception of the spectators about environmental futures.

Preliminary results: Researching the references and other practices that use future literacy and theatre of the oppressed to educate in non-formal spaces and about climate change has reinforced the potential of their intersection. In particular, the theatre of the oppressed and the future literacy action, whose pillars are the active involvement of the participants, collective dynamics, and the moldable necessary aspect of both practices, changes considering each group and its particularities. These similarities highlight, so far, the potential of the combination of artistic and scientific conception, as our initial hypothesis proposes. As research is ongoing, the conception, and exploration phases are taking place together, and so far, some interventions have been implemented. Among the interventions, there were practices of the theatre of the oppressed without connection to future literacy or climate issues, which highlighted how the peculiarities of each group greatly influence the progress of the dynamics. A two-day workshop with primary and secondary school teachers, who timidly introduced concepts of climate change, among other dynamics, highlighting the following games, which are still experimental. Machine game: an action where spectators are organised in a circle, and one by one, choosing a place at the centre of the circle, positioning their bodies in positions that first cross their mind, influenced by a specific spoken word. Some trigger words were environment, future, nature, and climate change. Once in this position, everyone froze, and then we analysed each pantomime, first from the outside point of view, the other member's perspective of that body image relates to the trigger word, and subsequently, asking the person herself what has in mind when decided on that position. Newspaper theatre: The organisers provided links to online newspapers centred on environmental related news. Then, the participants were told to form pairs or trios, pick information from one of the newspapers freely, read the news, and after talking with each other, present for the other spect-actors, without words, performing the theme of the information. Firstly, only with their bodies, and next, repeat the scene with body and sounds allowed (but not words). After each performance, those who watched the act had to discuss what they thought the scene was about and, collectively, decide on a suitable title. The initial news was revealed after all the presentations, discussions, and elections of the scene's titles. But the exciting thing is that this revelation of the new behind the scenes does not occur in the form of validating the debates or the group; the news is the trigger, but the centre of this game is how a lot of different nuances emerge from the subjectivity that each person projects in those scenes represented there by the others.

Preliminary conclusions: As said before, this is an ongoing project, so there are still steps and new explorations and interventions to happen, but, until now, the project shows promising evidence that our initial hypothesis was true, that the interdisciplinarity between science and

art, through creative processes is a powerful tool for raising awareness, inciting debates, reflections, and public engagement concerning climate action and fomenting the autonomy of individuals and collectives in building new futures.

Cylon Liaw
IEE-USP

Abstract Title: CCUS standardization mapping – The steps towards this strategic tool

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Abstract: This study explores the evolution of standardization frameworks, from early static models in the 2000s to recent developments that address strategic and tactical aspects. It identifies a persistent gap between these frameworks and the decision-making process for prioritizing standardization opportunities. To bridge this gap, a standardization mapping tool was developed. The tool adopts a technology roadmap-based standardization framework, integrating strategic elements (e.g., identifying relevant innovation activities, determining the need for standardization, and timing) and tactical considerations (e.g., methodology, location, and participants). Multiple-Criteria Decision Analysis (MCDA) techniques enhance the decision-making process. Preliminaryy findings indicate that this approach effectively addresses strategic and some tactical dimensions, reducing the framework's reliance on developer expertise. It serves as a versatile strategic tool for investigating and prioritizing standardization opportunities across different contexts.

Keywords: CCUS, Standardization, Database.

Introduction and Objectives: In the early 2000s, literature began to explore the evolution of standardization frameworks that outlined the various roles played by standards. These initial frameworks identified different facets of standardization, including types of technologies and other aspects of innovation activities. However, these early frameworks were static and did not address how standardization should evolve throughout the development of technology and industry lifecycles. Subsequent years saw advancements leading to the development of frameworks that focused on the processes of standardization, addressing strategic and tactical considerations. More recent developments have delved into the knowledge required to navigate transitions between critical anticipated innovation activities, thereby predicting potential

standardization needs for emerging technologies. Nevertheless, a gap persisted between these existing standardization frameworks and the decision-making process necessary for identifying and prioritizing standardization opportunities. The objective of this work was to bridge this gap by creating a tool for standardization mapping.

Methodology: The standardization mapping tool development included a literature review on standardization frameworks and decision-making techniques. After selecting an appropriate framework and suitable techniques, an application study was developed to prove the concept.

Preliminary results: The chosen approach for the standardization mapping tool is centred around a technology roadmap-based standardization framework. This framework integrates the strategic and tactical aspects of standardization into the existing technology roadmap model. Within the strategic dimension, the tool addresses questions such as identifying relevant innovation activities for standardization (S1), determining the necessity for standardization (S2), and establishing the optimal timing for standardization (S3). On the tactical front, the tool considers factors like how to proceed with standardization (T1), where the standards should be developed (T2), and who should actively participate in the standardization process (T3). To enhance the decision-making process for building this framework, it was incorporated Multiple-Criteria Decision Analysis (MCDA) techniques. This combined approach, which merges MCDA techniques with a technology roadmap-based standardization framework, was then applied to the Hydrogel Program. Its purpose was to prioritize standardization topics and determine the appropriate types of standards within that context.

Preliminary conclusions: All strategic dimensions and the first tactical dimension can be answered by coupling MCDA techniques with a technology roadmap-based standardization framework, reducing the reliance of this type of framework on the expertise of the framework developer. Additionally, it became a strategic tool which can be applied to different cases where standardization opportunities need to be investigated and prioritized.

Celso da Silveira Cachola
Universidade de São Paulo (USP) & Research Centre for Greenhouse Gas Innovation (RCGI)

Abstract Title: Geospatial Analysis and Clustering of Green Hydrogen Production and Consumption for Greenhouse Gas Emission Mitigation: A Case Study of Brazil

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Abstract: The work aims to mitigate climate change by harnessing the potential of green

hydrogen production and consumption to reduce greenhouse gas (GHG) emissions. As global temperatures increase and ocean warming reaches abnormal levels, the urgency of sustainable solutions becomes apparent. Hydrogen, particularly green hydrogen generated through water electrolysis using renewable energy, demonstrates remarkable potential in scientific realms. However, the efficient deployment of green hydrogen creates the need for strategic geospatial planning that considers both production and consumption aspects. This study utilizes Geographic Information System (GIS) tools and the K-means algorithm to analyze and cluster potential sites for green hydrogen production and consumption. By merging spatial and environmental data, a robust geospatial database is constructed, focusing on Brazil due to its substantial investments in hydrogen applications and clean energy leadership. The innovative integration of Geographic Information System and K-means algorithm enables the identification of optimal green hydrogen clusters, therefore contributing to greenhouse gas mitigation strategies. The primary research objective revolves around formulating and analyzing spatial clusters to address the dual aspects of green hydrogen, identifying the geospatial dynamics of the green hydrogen production and consumption. The central research question is: How can potential spatial green hydrogen clusters be formulated and analyzed to mitigate greenhouse gas emissions? The methodology employed in this study holds promise for adaptation and expansion to various contexts, offering valuable insights for future research endeavours beyond the Brazilian case study. The findings bridge a critical gap by considering both production and consumption in tandem, underscoring the importance of geospatial analysis in realizing the transformative potential of green hydrogen for a sustainable energy future.

Keywords: Hydrogen; Decarbonization; Geographical Information System (GIS); K-means; Brazil.

Introduction and Objectives: The escalating consequences of climate change, exemplified by record-breaking temperatures and increase ocean warming, underscore the urgent need for mitigating greenhouse gas emissions. The global pursuit of a low-carbon future has positioned hydrogen as a key player, offering versatile applications as a clean fuel, energy carrier, and raw material. Green hydrogen, produced through water electrolysis powered by renewable energy sources, emerges as a sustainable solution to mitigate climate change. While the importance of green hydrogen in the energy transition is recognized, its efficient production and consumption require strategic geospatial planning. The integration of Geographic Information System tools and data-driven methodologies can facilitate the identification of optimal production and consumption clusters. Despite several studies focusing on either the production or consumption aspects of green hydrogen. This work addresses this research gap by employing Geographic Information System and the K-means algorithm to identify and analyze spatial clusters for green hydrogen production and consumption, aiming to contribute to greenhouse gas emission mitigation. The primary focus is on investigating the establishment of spatial clusters for green hydrogen production and potential consumption, employing Geographic Information System tools and the K-means algorithm.

Methodology: The study constructs a geographic and spatial database integrating relevant data sources such as wind speed, solar irradiation, local greenhouse gas emissions, and more information. The Geographic Information System framework facilitates the analysis of potential clusters for both green hydrogen production and consumption. The K-means algorithm enhances this analysis, allowing for the efficient grouping of spatial data points.

Preliminary results: The outcomes of this study provide insights into the establishment and analysis of green hydrogen production and consumption clusters. Twenty clusters have been identified: eight hold potential for green hydrogen production using wind and solar energy sources, three emphasize the production of moss green hydrogen, i.e., hydrogen generated from biofuels, two are located in the Amazon region, two focus on both production and consumption, and finally, five clusters are potentials hydrogen consumers. By addressing both aspects simultaneously, the research contributes to a more holistic understanding of the geospatial dynamics of the green hydrogen. Moreover, the findings hold implications for shaping public policies, social perception studies or analyses, and guiding investments in the burgeoning green hydrogen sector.

Preliminary conclusions: This study underscores the importance of geospatial analysis and clustering in optimizing the production and consumption of green hydrogen for greenhouse gas emission mitigation. By utilizing Geographic Information System tools and the K-means algorithm, this research introduces a novel approach that paves the way for sustainable hydrogen consumption and offers a replicable methodology for further investigations. Ultimately, the integration of spatial and environmental dimensions is crucial for realizing the full potential of green hydrogen in reshaping the energy system.

André dos Santos Alonso Pereira; Karen Mascarenhas; Edmilson Moutinho dos Santos
University of São Paulo; RCGI; University of São Paulo

Abstract Title: Science Diplomacy and the Sustainable Development Goals: How RCGI may use it

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Abstract: Founded in 2016, the Research Centre for Greenhouse Gas Innovation (RCGI) is one of Brazil's leading hubs for advanced studies in the fields of energy and environmental issues,

contributing to numerous projects in those sectors. Consolidated on the main five research programs related to them, the institute began a new phase in 2021 aiming for more ambitious goals regarding climate change mitigation and energy-based solutions at a global scale. In doing so, RCGI may become an invaluable tool for Brazil's climate and energy policymaking. This could be achieved through Science Diplomacy initiatives, where Brazil (or its state of São Paulo, where RCGI is situated) can benefit from the centre's achievements to promote new energy solutions and technologies. To evaluate if RCGI's research is useful for broader Science Diplomacy actions, the present work will analyse if they follow the United Nations' Sustainable Development Goals (SDGs) program, which promotes an international cooperation agenda regarding global issues, like energy poverty and climate action. Through the application of a questionnaire during abstract submission for the 6th Energy Transition Research & Innovation (ETRI) 2023 Conference, we will observe RCGI's members' projects to verify how they are applying SDGs. Based on the data collected, our next step is to study how they are following Science Diplomacy actions, which in turn can help us determine how influential RCGI's projects are in the promotion of Brazilian science & innovation on energy and environmental concerns.

Keywords: Science Diplomacy; Sustainable Development Goals; RCGI, Brazil; Knowledge Diffusion

Introduction and Objectives: Research centres are the kind of institutions that can help themselves, as well as their host countries, benefit from science diplomacy (SD). The recent COVID-19 pandemic was an example of how nations and their laboratories raced to create vaccines and to get them diffused globally; two facts became apparent: Global issues can promote at the same time competition and cooperation between distinguished learning hubs; science is powerful for overcoming such harsh periods; and SD is essential in the strategy of institutions, and to accelerate scientific progress. Therefore, one can assume that scientific centres with more foreign connections and diplomatic presence, will have more advantages to enhance their work, while also creating more soft power tools for the nation they represent. According to the literature, soft power is how a country can persuade others to follow its policies without the use of coercion. This concept is mostly used to analyse national strategies, but it has been including private actors as beneficiaries of such a tool. Synergic effects are emphasized then as individual initiatives enhance their nation's own soft power. Unlike a governmental actor or a multinational company, a research centre usually lacks what authors would describe as essential factors of soft power, such as financial assets or coercive means. However, through the creation of a network with other agents like politicians, regulators, commercial agents and other centres, scientific institutes can build up their own relevance. Science diplomacy plays a leading role in that regard. A way to connect with the international community through SD is to pursue the Sustainable Development Goals (SDGs), an initiative of the United Nations to promote common objectives globally. It is assumed that implementing effective measures to promote the SDGs will generate a matrix of globally accepted and easily communicated achievements that will enhance science diplomacy potential of scientific

institutions. As an energy and environmental research centre, the Brazilian Research Centre for Greenhouse Gas Innovation (RCGI) has been consolidating itself as a major developer of ideas in the global climate debate, promoting policy suggestions, low-carbon technologies and more sustainable and acceptable ways for their implementation. Since its creation in 2015 within the University of Sao Paulo, the RCGI has been improving its actions in Science Diplomacy, including the systematic assessment of its contribution to the SDGs. We'll investigate in this paper how RCGI projects are intertwined with SDGs, pointing out how the alignment to the SDGs can improve RCGI's Science Diplomacy activism. We sustain that those actions are fundamental tools for the RCGI to grow its scientific relevance and to solidify itself not only as a preeminent global scientific institution in climate issues, but also as a significant asset to Brazil's policymaking in the climate debate and negotiations.

Methodology: The main objective of this work is to assess, through a questionnaire application at the ETRI 2023 Conference abstract submission process, which and how many SDGs are being impacted by the research under development at RCGI. We assume that submitted abstracts are early views of the researchers regarding the on curse works at RCGI. Not necessarily the involved scientists are fully aware of their potential impacts on SDGs, and on how their projects may help in RCGI's (and Brazil's) Science Diplomacy initiatives. The ETRI 2023 is the central scientific event that brings together RCGI members, as well as broader scientific and political communities. Therefore, the submitted abstracts to the scientific gathering allow us the perfect opportunity to collect early data regarding RCGI's effective commitments to the SDGs. Once the abstract submission process is finished, there will be early data available to analyse which of the seventeen SDGs are mostly applied for each project.
Previous research and analysis conducted by RCGI and applied to ongoing research projects at the centre have revealed that most research projects follow three major SDGs: numbers 7, 9, and 13 (respectively, affordable and clean energy; industry, innovation and infrastructure; climate action). At this paper, we will conduct an updated and comparative analysis in order to assess eventual major evolution in RCGI's commitments to the SDGs. The updated analysis will follow the same method adopted at the first study. Yet we will enjoy at ETRI 2023 an additional opportunity to also include a presential questionnaire for participants at ETRI 2023 to answer. We expect that the additional collected data can provide additional insights that will help us to suggest how the RCGI can develop more accurate Science Diplomacy initiatives and perform more impactfully towards the SDGs.

Preliminary results: As previously stated, it is important to note that, despite its growing endorsement on the bibliography and in the practices of scientific centres, the SDGs and Science Diplomacy might not be well known among scientists, which usually are too busy within their labs. Therefore, we believe that the major outcome of this work will be to verify whether the RCGI's researchers are already conscious of the broader potential perspective of their generated knowledge. For a centre with the bold mission of becoming one of the most prominent centres of excellence in climate issues and in proposing low-carbon technological solutions, the RCGI recognizes that each of its projects must align with the SDGs route. RCGI

projects must clearly contribute to overcome challenges linked to clean and sustainable energy, industry innovation and climate action. Such alignment is the most preponderant mechanisms to guarantee that each production coming out from RCGI will contribute to RCGI's self-proclaimed mission to promote technical innovations that can help reducing and mitigating the global GHG emissions.

Preliminary conclusions: At this present moment, we have no doubt that the ETRI 2023 will be an opportunity for RCGI to keep its growing momentum while also providing us with data to conduct our analysis regarding its employment in Science Diplomacy initiatives by Brazil's political and diplomatic classes, either from the federal government or the state of São Paulo, where the centre is located. Also, we can initially conclude that through applying the SDGs on its projects, RCGI members are already contributing towards Science Diplomacy.

Alberto J. Fossa
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Abstract Title: Standardization of Carbon Dioxide Capture, Transportation, Utilization and Storage (CCUS) – Recent developments at ABNT and ISO

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Abstract: Climate change poses a significant threat to the progress of present and future generations. In response, CCUS has emerged as a crucial tool for combating climate change, complementing other initiatives. This study focuses on establishing CCUS standards and explores the challenges in both international and national contexts. Preliminary findings reveal that the ISO CCS committee's scope, which presently excludes CCU, is under discussion but faces skepticism regarding the broad inclusion of CCU. A specialized standardization committee in Brazil has been established, taking significant steps in developing CCU-related standards. In conclusion, while international standardization discussions for CCU are yet evolving, Brazil has taken proactive steps in creating CCUS standards within its national context. This work highlights the importance of addressing CCUS within global and local standardization frameworks to combat the challenges posed by climate change effectively.

Keywords: CCUS, Standardization, Climate Change.

Introduction and Objectives: Climate change poses a significant threat to the progress of both present and future generations. Within this context, Carbon Dioxide Capture, Transportation, Utilization, and Storage (CCUS) has emerged as a crucial tool for addressing climate change. It operates in conjunction with other initiatives and strategic choices like transitioning to cleaner energy sources, enhancing energy efficiency, adopting sustainable practices, and more. There is a pressing need to delve into the specific aspects of CCUS within established standards, focusing on determining where CCUS standardization efforts should take place and how to forge strategic connections between the global standardization landscape and related Brazilian contexts. The primary objectives encompass advocating for CCU standards within existing international standardization forums and creating the initial set of national CCUS standards.

Methodology: The work is primarily conducted in standardization forums, each with its specific rules. In the international environment, the process involves interacting with experts and engaging in discussions within committees. In the national environment, developing a draft standard is based on international references and input from previously collected materials.

Preliminary results: Internationally, ISO/TC 265 is dedicated to CCS and has a working group (WG) for CO2-EOR, a CCU solution. Additionally, ISO/TC 265 has an ad-hoc group (AHG) discussing one technological route for CCU: carbon mineralization. Currently, ISO/TC 265 is discussing its scope, which excludes CCU, but experts are skeptical regarding the inclusion of CCU as a broad concept in the committee. Nationally, the Study Commission (CE) at ABNT/CB-038 on Environmental Management (CE-038.007.002 – Captura, Transporte, Utilização e Armazenamento de Dióxido de Carbono), formally established in June 2022, is already discussing its first CCU-related standards: three guidelines, the first on CCU terminology, the second on CCU technological routes, and the third on CCU-based products' carbon footprint.

Preliminary conclusions: Despite some specific initiatives, no international standardization environment has been established for discussing CCU standards. The current ISO committee dedicated to CCS has a scope that excludes CCU, and discussions to expand this scope to encompass specific CCU issues are underway. In Brazil, a dedicated standardization committee was established, a Study Commission focused on CCUS under the Environmental Management Brazilian Committee (ABNT/CB-038), and it is currently developing its first CCU-related standards.

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Abstract Title: Brazilian climate targets and the analysis of their alignment with Nationally Determined Contributions (NDCs)

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Abstract: In the 1990s Brazil began to show greater concern about the development of public policies, plans, and funding to try to mitigate environmental and climate problems. First discussions were established in 1992, in Rio de Janeiro, during the United Nations Conference on Environment and Development, when it was set the stabilization of greenhouse gas concentration (GHG) in the atmosphere as a goal. In order to achieve this goal Brazil signed three central commitments: the National Policy on Climate Change, the Paris Agreement, and the Nationally Determined Contribution (NDC) defined as voluntary commitments made by Brazil, within the scope of the United Nations Framework Convention on Climate Change (UNFCCC). Among these objectives we can find the reduction of GHG observing the deforestation rates and the integration of renewable sources to the energy matrix. Based on this assumption this article objective is to understand Brazil's climate targets and their alignment with the NDCs current situation. In order to reach this objective systematic research was carried out the CAPES Periodical, and USP Library. In this way it was possible to understand Brazilian NDCs current situation focusing on information from the Climate Observatory's Greenhouse Gas Emissions Estimating System (SEEG). The results show that Brazilian GHG emissions indicate that the country had in 2020 an increase of 9.5% of gross emissions while the global emissions reduction was almost 7%. Observing Brazil situation, it can be said that the country went against the rest of the world, having the highest percentage in emissions since 2006. Additionally, it was possible to conclude that Brazilian scenario for GHG mitigation presented negative results in 2020.

Keywords: public policies; Paris agreement; greenhouse gases; GHG.

Introduction and Objectives: In order to achieve this goal Brazil signed three central commitments: the National Policy on Climate Change, the Paris Agreement, and the Nationally

Determined Contribution (NDC) defined as voluntary commitments made by Brazil, within the scope of the United Nations Framework Convention on Climate Change (UNFCCC). Among these objectives we can find the reduction of GHG observing the deforestation rates and the integration of renewable sources to the energy matrix. This article objective is to understand Brazil's climate targets and their alignment with the NDCs current situation.

Methodology: In order to reach this objective systematic research was carried out the CAPES Periodical, and USP Library. In this way it was possible to understand Brazilian NDCs current situation focusing on information from the Climate Observatory's Greenhouse Gas Emissions Estimating System (SEEG).

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Preliminary conclusions: Observing Brazil situation it can be said that the country went against the rest of the world, having the highest percentage in emissions since 2006. Additionally, it was possible to conclude that Brazilian scenario for GHG mitigation presented negative results in 2020.

Alexandre de Barros Gallo
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Abstract Title: GHG mitigation through energy management – Current standardization approaches

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Abstract: Climate change is a significant sustainability challenge, with energy use responsible for three-quarters of anthropogenic greenhouse gas (GHG) emissions. Recognizing this, the international community sees energy management as crucial for improving energy efficiency and reducing emissions. Bridging energy management and GHG emissions reporting can enhance the credibility of emission reduction claims. This research examines GHG mitigation through energy management within standardization. This study employs an exploratory-

descriptive approach, engaging in a standardization forum on energy management. It explores how GHG emissions and energy management can integrate, using qualitative mono-method action research. Preliminary results highlight alignment opportunities between energy performance evaluation and GHG emission accounting, suggesting pathways to enhance standards. Preliminary conclusions identify two standardization movements: one global, converging GHG mitigation and energy management, and the other technical, supporting the former by aligning energy related GHG emission accounting and energy performance evaluation to improve reporting.

Keywords: GHG mitigation, Energy Management, Standardization.

Introduction and Objectives: Climate change stands as one of the foremost sustainability challenges in our era. The most substantial contributor to greenhouse gas (GHG) emissions, at three-quarters of the total anthropogenic emissions, is energy use. Recognizing this, the international community has pinpointed energy management as a crucial tool for addressing energy efficiency obstacles and fostering the integration of reduced demand and behavioral shifts within organizations' culture. By bridging the gap between energy management and GHG emissions reporting, we can enhance the credibility of claims regarding GHG emission reduction. This credibility is pivotal in the fight against climate change and the promotion of carbon neutrality. The primary objective of this research is to examine GHG mitigation through the lens of energy management within the framework of standardization.

Methodology: The research design adopts an exploratory-descriptive approach. It aims to investigate a specific environment, which is a standardization forum related to energy management, while fully engaging as a participant. The objective is to describe how two subjects, namely GHG emissions and energy management, can be integrated based on this exploratory experience. To achieve this, a qualitative mono-method action research strategy is employed, utilizing primary data obtained through observation. The research methods include elements of content and narrative analysis. The exploratory phase unfolds over time within the action research process. After completing the exploratory cycles, the descriptive phase provides a comprehensive analysis and a final standardization recommendation.

Preliminary results: From a standardization perspective, there are several alignment opportunities between energy performance evaluation with indicators and energy related GHG emission accounting. Core opportunities comprise adequate activity data and a suitable baseline, while other opportunities include, for example, definition of analysis' limits (boundaries). Implementing these opportunities could follow different paths, from informative annexes in standards covering these topics to a guidance standard.

Preliminary conclusions: Two specific movements were identified, as technical possible

movements and, more recently, as current standardization activities. The first movement is more global, converging GHG mitigation and energy management. The second one is more technical, aiming to support the first one, by combining energy-related GHG emission accounting and energy performance evaluation with indicators to overcome identified barriers and improve energy-related GHG emission reporting.

0911 – GHG20 (TV4)

Chairs: Renato Picelli – Guenther Krieger Filho

Glycon Pena de Souza Barros
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Abstract Title: *Development of labyrinth seal applied to pneumatic machines using the concept of intelligent materials to minimize leakage

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Abstract: Developing joints with complex geometries is necessary to reduce working fluid leakage in turbomachinery joints that use a labyrinth seal (LS) type shaft-rotor-stator sealing element. Depending on the variation in the flow of the working fluid, It is often necessary to modify the geometry of the LS teeth of the service part, depending on the composition of the fluid mixture, machine rotation, pressure, and workflow. In order to solve this difficulty, the use of intelligent materials becomes viable. This type of material changes its shape and properties in an insistent and controlled manner, allowing the joint to be manipulated. Shape memory alloy (SMA) has high resistance and slow response time, making it suitable for the intelligent seal in passive form to modify the seal teeth' geometry and create new configurations depending on the fluid mixture. Computational simulations were conducted for CH4 and CO2 gas to verify the ideal tooth inclination for each fluid composition. Nitinol alloy was used to tilt the teeth of the LS and thus obtain less fluid leakage. As a scientific contribution resulting from this research, the objective is to develop experimental tests to explore the concept of intelligent materials in the design of labyrinth joints applied to pneumatic machines, which will make it

possible to design a labyrinth-type joint with SMA Nitinol material, where the seal teeth may have the slope modified depending on the fluid mixture composition, such as CH4 and CO2. Modifying the teeth allows for greater joint efficiency, further reducing the leakage of CH4 and CO2 and thus reducing the climatic effects caused by the emission of these gases.

Keywords: Labyrinth seal, Turbomachine, Smart material, Nitinol.

Introduction and Objectives: There are several different types and geometries of labyrinth seal (LS) joints that allow a small leakage of the working fluid but are still inefficient when applied to certain types of gases (CO2 and CH4) and fields of applications in which there is a need to reduce further plus the leak in the labyrinth joint. To reduce leakage, the development of joints with complex geometries is necessary, but it is challenging to implement from the point of view of the electromechanical assembly and according to variations in the flow of the working fluid, often making it necessary to modify the geometry of the teeth. The labyrinth of the service part for each fluid mixture composition, machine rotation, pressure, and workflow. In order to solve this difficulty, the use of intelligent materials becomes viable. This type of material changes both its shape and properties in an insistent and controlled manner, allowing manipulation of the joint. Intelligent materials or “smart materials” are materials that have intrinsic and extrinsic capabilities to respond to stimuli and to activate their functions according to these changes (SIR, 2000). These are materials that have the ability to transform mechanical force and movement into another form of energy and vice versa. Among these materials, shape memory alloys (SMA – Shape Memory Alloy) stand out (MENDES et. al., 2003). Shape memory alloys (SMA) are a class of materials capable of recovering a previously known shape when their temperature increases. Under specific conditions, it has the ability to absorb and dissipate energy from different forms of cyclic loading (OLIVEIRA et. al., 2018). This material has two distinct phases and consequently different properties. One is the high temperature phase called AUSTENITIC (A) and the other phase called MARTENSITIC, which is low temperature. Martensite can be presented in two martensitic variants: Twinned Martensite (Mt) and Untwinned Martensite (Md). When heated without mechanical loading, the material transforms from twinned martensite to austenite. The starting temperature of the austenitic transformation (As) is the temperature at which this transformation begins, and the temperature (Af) is the temperature at which this transformation is completed. The reverse phase transformation occurs with the transformation from martensite to austenite with a reduction in temperature, with (Ms) being the temperature at which this transformation begins and (Mf) the temperature at which this transformation ends (OLIVEIRA et. al., 2018). The main effects that these binders present are known as SME (Shape Memory Effect) and pseudoelasticity (or superelasticity) (OLIVEIRA et. al., 2018).

Methodology: Through bibliographical research relevant to the topic, focusing on the following subjects: Labyrinth seals applied to air, CO2, and CH4 compressors; Smart materials; SMA material (Shape Memory Alloy); Scientific experiments. Carrying out tests on intelligent material called Nitinol for different lengths, diameters, and transformation temperatures to

evaluate the actuation force and fixings. Evaluation of different geometries of labyrinth seals that favor minimizing working fluid leakage and using SMA as an actuator. Assuming a mixture of CO2 and CH4 with a different composition from CH4 and CO2, evaluate the optimized seal configuration for fluid with a high composition of CH4 and a high percentage of CO2. Carry out experiments to evaluate possibilities of deformation of SL teeth using the Buckling system (Snap-Through), in which the snap-through is activated by a force caused by Nitinol. This system buckles when a load is distributed and applied. Once we have the joint design with SMA, we intend to manufacture a prototype of the joint using metal/polymer additive manufacturing using an existing printer at RCGI.

Preliminary results: Plate and wires made of intelligent material called Nitinol were specified and purchased. These materials were tested as actuators, using heat from an electric current source (Joule effect). Nitinol presents high mechanical resistance and is suitable for the intelligent seal in passive form. In addition to the activation test, training tests were carried out to evaluate the shape memory effect and tests for attaching wires to plates simulating an SL tooth. Conduct tests for fixing Nitinol wires using silver solder, spot welding, staples, ties, glue, and resin. Mastery in training Nitinol alloys to act when heat and electric current are applied. Tests to evaluate bi-stable systems ("buckling") such as a SL tooth. Parametric optimization of the SL considering a predominance of CO2 or CH4 in a mixture of these two gases to evaluate the best position of an SL tooth that would minimize leakage.

Preliminary conclusions: It was observed that the tooth inclination angles are different for CH4 and CO2. Using a bistable system such as an SL tooth driven by Nitinol and controlling the temperature, it may be possible to change the inclination in positions that offer a minor leakage of the working fluid.

Rômulo Luz Cortez
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Abstract Title: Compressor's Impeller Designs: Topology Optimization for Resonance Mitigation

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Abstract: In the field of compressor design, the impeller stands out as a crucial component. It serves as an essential element, yet its optimal performance is frequently challenged by resonance issues, especially when operating at nominal speeds. To address these obstacles, this research uses the TOBS-GT (Topology Optimization of Binary Structures with Geometry

Trimming) method. Through this methodology, we aim to elevate the impeller's stiffness and overall efficiency. These aspirations are more than academic, they hold direct implications for the real-world performance of compressors. The reduced susceptibility to resonance, as demonstrated through our research, can lead to fewer operational interruptions, minimized wear, and a consequent extension in the life cycle of the impeller. The Campbell Diagram served as a strategic tool throughout our investigation. By comparing its pre- and post-optimization versions, we were able to gauge the efficacy of our approach. The tangible shift of the impeller's design, shifting away from resonance-prone zones to a more stable operational spectrum using six frequencies simultaneously as constraints, was a proof of the versatility of the TOBS-GT method. In conclusion, the research underscores the promising horizons that the innovative TOBS methodology can achieve. With the resonance challenge being systematically tackled, the path becomes clearer for the development of compressors that are not only more efficient but also work within admissible mechanical stresses. These findings open new possibilities for further research and development in compressor design.

Keywords: Topology optimization, Compressor, TOBS, Natural frequency, Resonance.

Introduction and Objectives: In rotating systems, such as those present in turbo compressors, understanding and analysing vibratory behaviour are vital for safety and operational efficiency. By put our focus on modal analysis, it is possible to achieve more optimized designs where rotors can operate safely and efficiently across a broad spectrum of conditions. Modal analysis becomes fundamental in identifying vibration modes that could be excited under operational conditions. This project is intrinsically linked to the project: “Design Optimization and Experimental Evaluation of Centrifugal Compressors for CO2 and CO2-CH4 Mixtures in Supercritical Conditions”, from RCGI. Through this association, the aim is to develop rotors optimized for operations in specific conditions, particularly those "liquid-like" close to the critical point. In an academic panorama, the development and implementation of advanced approaches to deal with rotor design in complex scenarios is still a challenge, but it is essential to advance the boundary of knowledge and achieve more sophisticated and efficient engineering solutions. The TOBS (Topology Optimization of Binary Structures) method, already established method, continues to be a promising tool in this regard, allowing optimization based on Integer Linear Programming (ILP) and offering flexibility in defining constraints. With the challenges and uncertainties in mind, topological optimization of equipment, such as turbochargers, is extremely relevant. By exploring the design space, the objective is to increase operational efficiency, ensure safety against unwanted vibration modes and maintain stability levels within acceptable limits, thus leading to significant advances in the design and operation of such systems.

Methodology: This research centres on applying the TOBS method to effectively control the resonance of the impeller. At its core, TOBS employs mathematical programming to systematically determine the placement of solid or void regions within an optimization domain, guided by specific objective functions and constraints. In this study TOBS-GT, where GT refers

to Geometry Trimming, has been employed. This variant introduces a strategic distinction between the optimization and analysis domains. Specifically, while the optimization domain utilizes a fixed regular mesh, the analysis domain operates with a non-regular mesh. This methodology facilitates efficient calculations of sensitivities using COMSOL, especially in Multiphysics problems, which are subsequently remapped to the optimization domain. There, the ILP updates the design variables. To ensure a pragmatic approach and to guide the optimization process, frequency constraints were derived from the Campbell Diagram. This diagram elucidates the correlation between the rotor's rotation speed and its natural frequencies. Recognizing the impracticality of producing a Campbell Diagram for every iteration, the methodology was simplified. Effects such as the Coriolis force, gyroscopic effect, stress stiffening, and spin softening were excluded from the analysis. These adjustments, while considering the real boundary conditions of our 3D impeller model, resulted in a 100-fold reduction in computational time required for each iteration. To confer the algorithm with greater design freedom, the optimization domain was expanded, allowing for more flexible material removal decisions without compromising the final impeller's stiffness. Natural frequencies and their sensitivities to the design variables were then computed. By taking the average of these values across radial planes of the 3D impeller model, we set the stage for the next step: topology optimization in an axisymmetric domain. Thus, the design variables are updated in the axisymmetric plane and revolved around the rotor's axis for a subsequent analysis. This process continues until convergence is achieved.

Preliminary results: A comparison using the Campbell Diagram, both pre- and post-optimization, was crucial in evaluating our design approach. The results were clear: our updated impeller design successfully avoided zones known for resonance risks, leading to a more stable and dependable operation. Furthermore, a standout aspect of our methodology was the ambitious use of six frequencies as constraints. It's worth noting that in the field of topology optimization, leveraging multiple frequencies as constraints is a challenging task. However, our method demonstrated its robustness and effectiveness in efficiently dealing with these constraints, further highlighting the potential and versatility of the TOBS-GT approach in complex design scenarios.

Preliminary conclusions: Our research employing the TOBS-GT methodology has illuminated significant advances in the field of impeller design optimization, particularly in terms of resonance control. The comparison of the Campbell Diagrams pre- and post-optimization has provided solid evidence of the success of our approach. Not only does the refined impeller design effectively avoid traditionally problematic resonance zones, but it also leads to increase rotor lifetime and operational stability. The evidence from our work indicates that addressing resonance at the design phase, with a comprehensive and robust methodology, can mitigate challenges during actual operational phases of the impeller. Furthermore, the decision to incorporate six frequencies as constraints has showed the versatility of the TOBS-GT method, demonstrating its potential for such applications in design scenarios. This research

not only offers solutions to existing challenges in compressor design, but also presents the TOBS-GT method as an alternative for solving complex problems.

Shahin Ranjbarzadeh
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Abstract Title: Multi-objective function topology optimization design of labyrinth seal

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Abstract: Labyrinth seals are the most popular and the oldest mechanical sealing solution in the industry and play a vital role in the prevention and reduction of fluid emission. In the last decades, the improvement of the Labyrinth seal in multi-stage pumps and compressors attracts a great attention. Due to the very high number of geometrical parameters (e.g., seal cavity depth, seal tooth thickness and tooth tip clearance) and difficulties related to determining their effects on labyrinth seal performance, the Topology Optimization is a feasible approach to achieve the best design with the highest efficiency. Thus, this work presents a Topology Optimization formulation for design the labyrinth seal by using a 2D swirl flow model. The model is developed based on the Navier-Stokes equation to consider an axisymmetric flow with flow rotation around the shaft (fluid flow in labyrinth seal), and a multi-objective function is defined in order to maximize the of dissipation energy in fluid domain and maximize the velocity at selected points. The Topology Optimization formulation with a 2D swirl flow model is implemented in COMSOL Multiphysics (based on the finite element method) and solved using Sparse nonlinear OPTimizer (SNOPT) solver. Post-processed results, e.g. Topology optimization design, fluid flow, and pressure contour, is presented. The results indicate the reduction of leakage in optimized configurations of labyrinth seal compared to traditional configurations.

Keywords: Topology Optimization, Swirl, Labyrinth seal.

Introduction and Objectives: Labyrinth seals are the most popular and oldest mechanical sealing solution in the industry and play a vital role in the prevention and reduction of fluid emission. In the last decades, the improvement of the Labyrinth seal in multi-stage pumps and compressors attract great attention. Due to the very high number of geometrical parameters (e.g., seal cavity depth, seal tooth thickness and tooth tip clearance) and difficulties related to determining their effects on labyrinth seal performance, the Topology Optimization is a feasible approach to achieving the best design with the highest efficiency.

Methodology: Thus, this work presents a Topology Optimization formulation for designing the labyrinth seal by using a 2D swirl flow model. The model is developed based on the Navier-Stokes
equation to consider an axisymmetric flow with flow rotation around the shaft (fluid flow in labyrinth seal), and a multi-objective function is defined in order to maximize the of dissipation energy in fluid domain and maximize the velocity at selected points. The A Optimization formulation with a 2D swirl flow model is implemented in COMSOL Multiphysics (based on the finite element method) and solved using Sparse nonlinear OPTimizer (SNOPT) solver.

Preliminary results: Topology optimization creates mechanical restrictions in the flow path with an inclination toward the inlet flow. Topology optimization with a multiobjective function considering dissipation energy at the domain and velocity at selected points gives us the ability to choose the locations of the minimum gap inside the labyrinth seal. Furthermore, more points generate more mechanical restrictions.

Preliminary conclusions: Topology optimization is a robust method for designing the labyrinth seal and obtaining new configurations to reduce leakage.

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Abstract Title: Gas-like behavior constraint for s-CO2 Compression Train Optimization

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Abstract: The rising importance of Carbon Capture, Utilization and Storage (CCUS) industry due to global warming has increased the development of new technologies. The centrifugal compressors train is an essential system required for the storage of supercritical CO2 (s-CO2) into oil wells, a process known as Enhanced Oil Recovery (EOR), in which the pressurized fluid works above the critical point and close to the widom-line. The optimization proposed uses a Gas-like Behavior Margin (GBM) to avoid high variations of thermodynamic properties on the compression process close to widom-line, avoiding transcritical phenomena that can cause damage to the equipment. Moreover, the Acceleration Margin to Condensation (AMC) and Mach number at the throat are imposed as constraints as well. Finally, a CFD model for the

last stage of compression was built, which demonstrated good agreement with 1D model, proving the validity of using the methodology developed herein, as a fast and low-cost way to obtain a Preliminary geometry for centrifugal compressors of EOR compression systems.

Keywords: Carbon Capture, Utilization and Storage; Enhanced Oil Recovery; Centrifugal Compressors; Supercritical CO2; Gas-like Behaviour Margin.

Introduction and Objectives: The impact of Greenhouse Gases (GHGs) on the world's environment has driven the scientific community to pursue a reduction of emissions through renewable energy sources, energy efficiency improvements and atmosphere mitigation of CO2, which can deliver important reductions in world's total emissions through Carbon Capture, Utilization and Storage (CCUS) technologies, perhaps reaching negative emissions. The most economically viable type of geological storage of the CO2 used by the oil and gas industry is the reinjection of CO2 into oil fields for additional production. That process is called CO2 Enhanced Oil Recovery (CO2-EOR). The compression systems used in EOR are often multi-staged with intercoolers between them to avoid high temperatures. As compressors consume most of the energy in the chain, they must be highly efficient, consuming the lowest possible power to deliver the desired outlet pressure. Therefore, optimization of these compression trains is essential for ensuring a financially competitive project, reducing its consumed power. However, the optimization of compression systems presented in literature so far, do not consider geometrical constraints and fluid flow phenomena in the equipment as shock waves, gas-like behaviour and condensation. Thus, a well-established one-dimensional (1D) model is used to represent the aforementioned fluid flow phenomena in centrifugal compressors to design a viable compression train, combining high thermodynamic performance with adequate fluid flow behaviour, allowing the actual feasibility of the resulting model. The centrifugal compressor of the last stage of CO2 reinjection, works in a supercritical state, near the critical point, which may difficult the CFD model convergence due to high property variations. Moreover, the phenomenon of the transcritical phase is still not fully understood by the scientific community, which can cause damage or jeopardize the machine's performance. The experimental data at this level of pressure led the researchers to circumvent that issue without well-defined criteria. Therefore, the proposed Gas-like Behaviour Margin (GBM) can avoid undesirable transcritical flow phenomena, ensuring that the s-CO2 compressor operates at the gas-like region. This approach combines reductions in power consumption with physical feasibility, which takes the s-CO2 compression systems optimization to the next level.

Methodology: The strategy applied in this analysis is to fix a number of compression stages identified in literature (four compressors), representing each stage through the implemented 1D model to perform an optimization procedure, which aims to reduce the total power consumed by the whole train, respecting the presented constraints: Throat Mach Number, Acceleration Margin to Condensation (AMC) and Gas like Behaviour Margin (GBM). Finally, a CFD model is built to verify the predictability capacity of 1D model optimization strategy.

Preliminary results: The insertion of the constraints on the optimization procedure through 1D modelling was able to avoid undesired fluid flow phenomena related to s-CO2 centrifugal compressor train system such as shockwaves, condensation and ensured gas-like behaviour, which was able to provide a feasible compression system at the gas-like region, respecting all initial design constraints and goals. The optimization procedure finds the optimal configuration of the compression system close to widom-line, consuming less power to increase the pressure to the desired level at the outlet of the 4ª stage compression. Clearly, the GBM prevents the reduction of the fourth stage PR to keep the compression system at the gas-like side on T-s diagram, blocking the fourth stage from crossing the widom-line toward liquid-like region during the optimization procedure, which is undesired due to high s-CO2 thermodynamic properties variations that can cause damage to the equipment. Finally, the CFD phenomenological analysis performed at the fourth stage of compression verified the effectiveness of the one-dimensional optimization by corroborating that no condensation was found since the comparison of the Mach number at the machine's throat is lower than the AMC level. In fact, the maximum Mach number at the throat estimated through the 1D code is 0.69, which is corroborated by the CFD results that estimated a maximum value of 0.68 at the leading-edge shroud. Since AMC value for this machine inlet condition is 0.71, condensation is not expected to occur. The low differences between 1D and 3D approaches indicate that the methodology presented can design robust centrifugal compressors operating at the supercritical state of the CO2 while maintaining the gas-like behaviour. Moreover, CFD models can better predict total power consumption than the 1D loss models since turbulence, recirculation and swirl are better addressed due to their tridimensionality nature. The total power consumption found by CFD model is 4.94% higher than 1D model. Nevertheless, the 1D methodology remains an excellent tool to provide an initial centrifugal compressor design.

Preliminary conclusions: The Gas-like Behaviour Margin (GBM) for supercritical fluids was able to circumvent the uncertainties of operating on the supercritical transitional region, ensuring suitable CFD convergence and physical reliability that is not contemplated by a traditional thermodynamic analysis. The total power consumed predicted by CFD modelling is higher than the 1D due to three-dimensional loss phenomena. Nevertheless, a good agreement between numerical approaches is still verified, ensuring that the 1D code approach is robust for preliminary designing of EOR compression systems. Overall, the construction of an experimental facility of centrifugal compressors operating with s-CO2 could provide better losses prediction for 1D model of supercritical fluids, improving the whole analysis taken herein.

Alberto Lemos Duran
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Abstract Title: Topology optimization method applied to the design of compressor impellers for supercritical CO2 considering turbulent compressible flow and resonance frequency constraint

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Abstract: Excessive emissions of greenhouse gasses (GHG), such as methane (CH4) and carbon dioxide (CO2), have negative consequences on the environment, as a result, strategies such as capture and storage (CCS) have been developed to try to control them, where one of the stages of the process involves the compression of CO2 above the critical point. The operating efficiency of compressors can be improved by reducing the rate of gas leakage through the seals and increasing the energy transferred from the impeller to the fluid. This work focuses on the design of compressor impellers for supercritical CO2 using topology optimization techniques in order to increase the compression efficiency. Topology optimization offers more freedom when compared to shape and parametric optimization, due to its non-intuitive solutions generated from determined initial domains. With the recent advances on additive manufacturing technologies, now it is possible to manufacture complex designs that before seemed infeasible. The solution of the fluid problem will be approached by applying the Favre mean to the Navier-Stokes equations, considering the Brinkman penalty and using the Wray-Agarwal formulation as a turbulence model and the CoolPROP software for the calculation of the real fluid properties. The optimization problem will be approached by formulating an objective function based on the vorticity and the energy dissipation and considering constraints of volume and resonance frequency, which is a common problem in rotating machines. The calculation of the sensitivities will be performed using the automatic differentiation of the FEniCS dolfin-adjoint library. As in this work a formulation based on topology optimization of binary structures (TOBS) will be used, with discrete design variables, the optimization problem will be solved by integer linear programming (ILP). At the end of the work, it is expected that the developed topology optimization formulation will contribute to the design of compressors for supercritical CO2.

Keywords: topology optimization; design of compressor impellers; compressor for supercritical CO2; resonance frequency in rotating machines; automatic differentiation

Introduction and Objectives: Excessive greenhouse gas (GHG) emissions have negative environmental consequences, including pollution, wildlife extinction, and global temperature rise. A major contributor to these emissions is carbon dioxide (CO2), primarily originating from coal, natural gas, and oil sources. In response to this critical issue, various projects has beem initiated, such as Carbon Capture and Storage (CCS), which involves capturing CO2 emissions

from major sources, compressing, transporting, and securely storing them. However, compressing CO2 for transport and storage, especially over supercritical conditions, presents formidable challenges. To effectively combat climate change, it is needed to study and develop technologies that not only reduce GHG emissions but also optimize resource utilization. This research seeks to address this pressing concern by applying topology optimization techniques to maximize the compressibility efficiency of compressors for supercritical CO2, thereby enhancing the energy transfer from the impeller to the fluid. Supercritical CO2 conditions are unusual and demand specific development and improvements to make CCS processes economically viable, efficient, and capable of mitigating GHG-related issues. In such conditions, the fluid behaves as compressible due to high velocities and property variations. Incorporating compressibility into the problem increases system complexity and the complexity of finding a solution. However, Computational Fluid Dynamics (CFD) techniques enable precise study of fluid behaviour within rotating machines, with a particular focus on compressor design. Several studies have employed the finite volume method and impeller sector modelling to address these challenges (Mangani, Casartelli, and Mauri, 2012; S. G. Kim et al., 2014; Ameli, Turunen-Saaresti, and Backman, 2018; Ameli, Afzalifar, et al., 2018; Romei, Gaetani, and Persico, 2022). However, herein is adopted topology optimization. This approach offers exceptional flexibility in designing mechanical components, allowing the creation of new contours and the elimination of existing ones, leading to non-intuitive solutions. Recent research has explored the application of topology optimization methods to fluid flow, resulting in significant advancements and the development of efficient and adaptable methodologies (Sa, Okubo, and E. C. Silva, 2021; Romero and E. C. N. Silva, 2014; Sa, Yamabe, et al., 2021; Borrvall and Petersson, 2003; Yoon, Jensen, and Sigmund, 2007). This research is the continuation of the scientific work developed in the area of topology optimization applied to flow. The main goal is to develop topology optimization formulations that facilitate the design of compressors for supercritical CO2, considering turbulent compressible rotary flow and resonance frequency as a constraint.

Methodology: The solution of the fluid problem will be approached by applying the Favre mean to the Navier-Stokes equations. The Brinkman penalty will be added to the momentum and energy equations. The Wray Agarwal turbulence model will be used as it is a model with just one equation free from the calculation of the wall function. The CoolPROP software will be used for the calculation of the real fluid properties. The optimization problem will be approached by formulating an objective function based on the vorticity and the energy

dissipation and considering constraints of volume and resonance frequency to ensure structural stability. The calculation of the sensitivities will be performed using the automatic differentiation of the FEniCS dolfin-adjoint library. As in this work a formulation based on topology optimization of binary structures (TOBS) will be used, with discrete design variables, the optimization problem will be solved by integer linear programming (ILP).

Preliminary results: Implementations were carried out to solve the problem directly in the

OpenFOAM finite volume solver, problems in laminar and turbulent steady state were solved and the calculation of the objective function was implemented. The study of sensitivity calculation using the FEniCS dolfin-adjoint library continues, with this it will be possible to perform topology optimization. In parallel, the original OpenFOAM solvers were edited, to introduce the material model into the equations that govern fluids, and new equations were added to allow calculating fluid properties from property tables. In the future this will be the way to include of CoolPROP in the topology optimization solver.

Preliminary conclusions: By applying topology optimization to fluid flows considering objective functions based on energy dissipation and vorticity, it was possible to eliminate the sharp corners of cavities in internal flow, in order to obtain the optimal path for the flow, reducing losses. It was seen that the results obtained with the use of software to calculate the real properties of fluids are close to those obtained by equations such as Peng-Robison, therefore it will be evaluated which approach is more efficient in time and complexity to be introduced in the optimization.

José Guedes Fernandes Neto
University of São Paulo

Abstract Title: Soil carbon stocks dynamics during tropical forest restoration in Atlantic Forest

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Abstract: Restoring forests can increase soils carbon stocks compared to previous agricultural uses and contribute to the capture of carbon dioxide from the atmosphere. However, there is little understanding of this process throughout the recovery of native forests, especially in large-scale studies. The objective of this work is to understand how different forest restoration methods contribute to increasing soil carbon stocks in the state of São Paulo. To this, in this study we evaluated soils in chronosequences in different types of forest restoration in São Paulo. We established approximately 700 plots of 30 x 30 m distributed throughout the State, in order to obtain a wide variation of biophysical conditions. We collected the surface layer of soil, from 0 to 10 centimetres, for various physical, chemical and biological variables to understand how they have behaved throughout these restoration methods, in different climatic and soil conditions. Forest ages were determined using the AVOCADO (Anomaly Vegetation Change Detection) algorithm. Statistical analysis was performed using a linear model in which carbon content was a function of age, type of restoration, clay content, soil density, cation exchange capacity and above-ground biomass. We performed the normality and homoscedasticity test of

the variables and used the Box-Cox transformation to adjust the data to the assumptions of the linear model. Abandoned monocultures are those with the highest average soil carbon stock for the surface layer (0 to 10 cm) with 32 MgC/ha, followed by natural regeneration (25.9 MgC/ha), active restoration (21.6 MgC/ha) and agroforestry systems (17.8 MgC/ha). We analyzed soil carbon stocks in relation with age, restoration methods and clay content, separately. After that, we integrated them into a linear model, and we found a significant p (p = 2.2-16) and an R^2 of 34.5%. When we included some variables on this model (CEC, soil bulk density and AGB), we found a strong significant p-value (p = 2.2-16) and a R^2 (0.80 or 80%). The results of this work may contribute to a better understanding of soil ecosystem services in forest restoration and, in this way, may impact the development of public policies.

Keywords: natural regeneration, tropical forest succession, active restoration, soil recovery, climate change mitigation.

Introduction and Objectives: The state of São Paulo has undergone an intense process of transformation over the last 200 years (Victor et al., 2005), which resulted in the early 1990s in a vegetation cover of 13.4% of the original total. Despite this, native vegetation in this state has increased in the last 30 years and reached approximately 23% of its area (São Paulo, 2022), mainly through the expansion of natural regeneration and active restoration (Rosa et al., 2021; Rezende et al., 2018).

In this heterogeneous landscape, natural ecosystems are inserted and contribute to the generation and maintenance of ecosystem services that are essential for the functioning of human society. The recovery of native vegetation cover also contributes to the generation of these services and this needs to be better understood, especially the services generated by the soils. It is important to understand how soil properties, from those that are inherent to this to those that change with management, are related to ecosystem functions and how they provide ecosystem services to society (Adhikari & Hartemink, 2016). In general, studies in forest restoration have given little emphasis to soil attributes. Mendes et al. (2018) analyzed 159 forest restoration monitoring studies and noted that only 41% of these authors collected soil data. Among the many variables used, soil organic carbon (SOC) is of central importance considering its correlation with several chemical, physical and biological variables, as well as its importance in the context of climate change. SOC is influenced by clay content and soil mineralogy, aggregate formation, land use history, nutrient availability and biological activity (Veldkamp et al., 2020). Among the actions to mitigate climate change and reduce greenhouse gases in the atmosphere, there is a growing focus on the potential of carbon storage soils. There is an engagement of the agricultural sector to improve production practices and thus store carbon in the soil, so that it can enjoy the carbon credit market (Popkin, 2023). Considering this, it is essential to understand how forest recovery contributes to this acquisition of carbon in the soil, given that this activity has high potential to recover the stocks of conserved forests. Associated with this, different restoration techniques, from active restoration to natural regeneration, may have different carbon stocks over time given the methods used for this. However, it is necessary to understand how the incorporation of aboveground biomass will create a carbon cycling

system so that the balance of this element in the soil becomes positive. The objective of this study is to analyse how the stock of organic carbon in the soil behaves in the surface layer during forest restoration in the Atlantic Forest in the State of São Paulo.

Methodology: The collection area of this work is in the state of São Paulo and has 690 plots, in which 405 plots are allocated in forest restoration areas in this state. This research is part of the thematic project "Understanding Restored Forests for benefiting people and Nature - NewFor", funded by the São Paulo Research Foundation (FAPESP) and the Netherlands Organisation for Scientific Research (NWO). NewFor grouped forest cover into eight categories according to a gradient determined by the reference ecosystems, which are forest or agricultural use. These types of land use are as follows: 1) Agroforestry Systems (SAF); 2) Monocultures in use; 3) Pasture and agricultural areas; 4) Abandoned monocultures (MonoAban); 5) Restoration plantations (Rest); 6) Natural regeneration (Reg); 7) Degraded Forest remnant; and 8) Conserved Forest remnant. For this work we analysed categories 1, 4, 5 and 6 as they are related to the forest restoration process. The plots have dimensions of 30 x 30 meters, or 20 by 45 meters (totalling 900 m^2), and were installed in order to avoid the edge effects. A forest inventory was carried out, in which all trees above 5 centimetres in diameter breast height (DBH) were measured as well as their heights. From this, it was possible to determine the aboveground biomass (AGB) through the equation of Chave et al. (2014). The soils were collected through deformed and undisturbed samples. For the deformed we collected with an auger three simple samples in the depth of 0 to 10 centimetres in order to generate a composite sample of the plot. From this, several parameters are analysed, among them carbon, texture, cation exchange capacity (CEC). The undisturbed samples were performed with a sampler and sampling rings at a depth of 0 to 10 cm, and the bulk density was determined in the laboratory. Soil carbon was determined by dry combustion at 1000 °C with LECO TRuspec CNHS. The carbon stock was calculated using the equivalent mass method, in which the soil density of conserved forests was used as a reference for comparison with other land uses. The granulometric analysis was carried out by sieving a portion of this collection to determine the sand content. The remaining material, composed of silt and clay, was placed in glass cylinders with water for decantation. After this process, the clay and silt contents were determined according to the mass of their fractions. The ages of the plots were identified using the AVOCADO (Anomaly Vegetation Change Detection) algorithm. The data were analysed using linear models, in which the carbon stock per plot was a function of age, type of restoration, CTC, soil density and AGB. As the data did not meet the prerequisites of normality and homoscedasticity, they were transformed using the Box-Cox method.

Preliminary results: Based on data on soil carbon stocks for each plot corrected by the equivalent mass of forest remnants at each site, we analysed the behaviour of these stocks over the time of forest succession, types of restoration, clay content, aboveground biomass, bulk density and CEC. Initially, we sought to understand some isolated relationships between these variables and the carbon stock in the soil and then understand the interactions between them. Abandoned monocultures are those with the highest average carbon stock values for the surface

layer of the soil (0 to 10 cm) with 32 MgC/ha, followed by natural regeneration (25.9 MgC/ha), active restoration (21.6 MgC/ha) and SAFs (17.8 MgC/ha). We performed an ANOVA between the types of restoration and their C stocks and there is a significant difference between them ($p = 1.81\text{-}9$). The test Tukey a posteriori details these differences between treatments and only active restoration and natural regeneration do not have differences between their C stocks. When analysing the carbon stock for all types of restoration together over time, we observed a significance ($p = 0.0006$) of the relationship, but with a low R^2 (0.04 or 4%). That is, in general, the stock of C in the soil increases over time. Then, we performed the analysis of this stock with the amount of clay in the soil and found a significant positive relationship ($p = 1.6\text{-}12$) and R^2 of 0.14 or 14.3%. That means that the higher the clay content in the soil, the higher the carbon stock, an expected relationship for these data. With these Preliminary analyses, we created a model in which the age of the forests, the types of restoration and the clay content were related to the C stock in the soil. We found a significant p ($p = 2.2\text{-} 16$) and a R^2 of 34.5%. The significant interaction found was between forest age and active restoration. Finally, we created a linear model with more variables, in which we included, in addition to the variables described in the previous model, the CEC, soil bulk density and AGB. This model obtained a significant p value ($p = 2.2\text{-}16$) and a R^2 of 0.80 or 80%. Active restoration was the type of forest that showed significant interactions with virtually all variables. With these results, we intend to refine the analyses to follow up the discussion and elaboration of a scientific article on the factors that influence the increase of carbon stocks in the surface layer of the soil in forest restoration areas in the State of São Paulo.

Preliminary conclusions: This research presents an extensive database from a significant collection effort in order to contemplate a wide biophysical gradient, vegetation types, soils and forest restoration strategies in the State of São Paulo. In these preliminary analyses, we have observed important patterns for the recovery of carbon stocks in the soils of the areas under forest restoration process by different methods. From this, we intend to carry out new analyses involving the patterns of recovery in the first twenty years of forest restoration, given a series of previous studies that indicate a rapid increase of carbon stocks in the soils in this period. In addition, we intend to understand what happens to carbon stocks in the soil after the first 20 years of restoration. We also need to include in the analysis the comparison with the reference areas, from forests to agricultural uses, in the sites studied to evaluate how these stocks are behaving along this gradient of land uses. It is essential to recognize the importance of collecting data in deeper layers of the soil, up to 1 meter deep, to have a broader view of carbon stocks in the soil and their processes throughout forest recovery. However, this project chose to invest in the installation of hundreds of plots in the state of São Paulo and it was not possible to carry out so many samples on the same plot. Understanding what happens to soil carbon stocks during forest succession is of great importance for the science and practice of forest restoration. Deepening these analyses can contribute to the formulation of public policies and draw the attention of a growing market related to carbon storage in terrestrial ecosystems. Currently, carbon market efforts are focused on gaining above-ground biomass and little is said about soil carbon stocks in forest restoration.

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Abstract Title: Large eddy simulation of a dimethyl ether turbulent jet diffusion flame

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Abstract: The main objective of this work is to obtain numerical solutions for a turbulent jet diffusion flame of dimethyl ether (DME) in a burner. Thus, a mathematical model based on the combustion process is formulated and solved in a three-dimensional computational mesh, under the assumption of flow at low Mach number. This model includes equations of continuity, momentum, mixture fraction, enthalpy/temperature and concentration of chemical species, which generate a highly complex system of nonlinear partial differential equations. The equations for these chemical species were derived from an adapted DME oxidation mechanism consisting of sixteen reactions, each with their respective rate parameters, involving a total of eighteen chemical species. The discretization of the model in the mesh is done using the Finite Difference method, while the turbulence treatment is done using the Large Eddy Simulation (LES) methodology. Using LES, the largest turbulent structures present in the flow are calculated directly on the mesh, while the smaller ones are treated indirectly by submesh models. The resulting algebraic system for flow is then solved by the Simplified Runge-Kutta method, while the chemical part of the model is integrated using Rosenbrock's semi-implicit method. For validation purposes, the numerical results obtained are compared with experimental data from Sandia National Laboratories and show good agreement. These results provide important information related to the mixing and reactions involved in the combustion of DME.

Keywords: DME jet diffusion flame, Large Eddy Simulation, Finite Difference, Simplified Runge-Kutta, Rosenbrock.

Introduction and Objectives: Dimethyl ether (DME) is the simplest ether, a fuel whose molecular structure consists of two methyl groups bonded to an oxygen atom, expressed by the chemical formula CH3OCH3. Its production occurs mainly from natural gas, coal and biomass — a factor that makes it a (bio)fuel with high production availability. Despite being a highly flammable volatile gas at normal atmospheric conditions, it can be easily liquefied under low pressure (about 0.6 MPa) and can be used as a fuel in compression-ignition diesel engines with little engine modifications. Compared to traditional petroleum fuels, DME is a high efficiency fuel with reduced emissions of nitrogen oxides and particulate matter, due to a low carbon-to

hydrogen ratio and absence of carbon-carbon bonds within its molecular structure. The characteristics that make DME a good alternative fuel increase the relevance of studies on its combustion. In this context, the objective of this work is to numerically investigate the reactive flow related to DME turbulent jet diffusion flames. For validation purposes, the results obtained through a numerical simulation are compared with experimental data from the Sandia National Laboratories, more specifically those related to the Sandia DME D flame. In this diffusion flame, DME is injected into the burner from a central tube with diameter d = 7.45 mm, and a pilot annulus with inner and outer diameter of 8 mm and 18.2 mm, respectively, is used to stabilize the flame. To enable combustion, a co-flow of air, at ambient conditions, of 25.4 cm by 25.4 cm is injected and surrounds the pilot jet. The Reynolds number resulting from this flame is approximately 29,300.

Methodology: The mathematical model of the Sandia DME D flame developed in this work is based on certain assumptions. Inside the burner, it is assumed that the flow has a low Mach number, the pressure remains nearly constant, heat losses through the walls are negligible and radiation contribution is negligible as well — reasonable assumptions for typical burner conditions. The model comprises equations of continuity, momentum, mixture fraction, temperature and chemical species concentration. These chemical species equations were derived from an adapted DME oxidation mechanism consisting of sixteen reactions, each with its respective rate parameters, involving eighteen chemical species. Once the computational mesh of the burner geometry is generated, the model is discretized using the Finite Difference method, with turbulence handled using the Large Eddy Simulation (LES) methodology. In LES, the larger turbulent structures in the flow are directly calculated on the mesh, while the smaller ones are indirectly treated through submesh models. The resulting algebraic system for the flow is then solved using the Simplified Runge-Kutta method, while the chemical part of the model is integrated using Rosenbrock's semi-implicit method. The described mathematical model and solution procedure are computationally implemented in Fortran 90. Using this code, numerical results for the Sandia DME D flame are calculated and compared with experimental data from Sandia National Laboratories at six axial positions (x/d = 1, 5, 7.5, 10, 20, and 40) and at one radial position (on the centerline of the burner), covering the entire flame composition space. Here, the axial direction (x-direction) corresponds to the direction in which the fuel is injected into the burner.

Preliminary results: In general, our numerical simulation resulted in a good level of agreement between the numerical and experimental data for the mixture fraction and temperature of the Sandia DME D flame. We observed that the mixture fraction stays close to 1 for $x/d < 10$, indicating a low level of burning due to little mixing between fuel and oxidant in this region. Consequently, the temperature remains approximately constant with no significant heat release. For $x/d > 10$, fuel oxidation begins to occur more intensely at the jet centerline, causing the mixture fraction curve to decrease and the temperature curve to rise. Due to the reasonable results obtained for temperature and the effectiveness of the combustion kinetic mechanism used in the simulation, we obtained good numerical results for four main products: carbon

dioxide (CO2), carbon monoxide (CO), water (H2O) and molecular hydrogen (H2). Among these chemical species, CO concentration proved to be the most challenging to approximate with numerical results. Unlike the other species, CO production increases considerably from the jet outlet nozzle to the final part of the flame, where high temperatures prevail. This is because CO is naturally highly sensitive to temperature and has its production peak at temperatures greater than 1500 K. Naturally, the largest discrepancies between numerical and experimental data occurred at regions of the flame far away from the jet outlet nozzle (x/d = 20 and x/d = 40). This happens because the jet flame structure starts with a potential zone of 1 to 10 diameters length and ends with a turbulent plume, which is very difficult to simulate using conventional numerical techniques, including Reynolds Averaged Navier-Stokes (RANS) and LES.

Preliminary conclusions: The numerical simulation carried out in this study for the Sandia DME D flame provided important theoretical-practical relationships inherent to combustion. Combined with an efficient method for solving flow equations, the LES methodology proved to be a viable and effective approach for the flame simulation, with a relatively low computational cost. Strong similarity was observed with experimental data using this technique in mean profiles for axial locations with x/d < 10. The most significant differences persisted at x/d > 20, an area of the flame characterized by high turbulence, and therefore naturally more challenging to simulate. As a part of our future efforts to improve our research, we intend to perform numerical simulations of diffusion flames of DME with the addition of H2, analysing the energy efficiency of the mixture and its ability to reduce greenhouse gas emissions.

João Baptista Dias Moreira
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Abstract Title: Integer Variable Topology Optimization applied to Full Waveform Inversion for salt reconstruction.

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Abstract: Full Waveform Inversion (FWI) is a fundamental tool in the reconstruction of velocity models involving complex geological formations such as salt bodies. A critical aspect of this process is the precise delineation of subsalt structures. The methodologies for accurately identifying and reconstructing these regions have been evolving in the last few years. Existing approaches often struggle with the sharp contrasts and high acoustic velocities associated with salt bodies, making it more difficult to estimate the base-of-salt (BoS) region compared to the top-of-salt (ToS). This study seeks to address this challenge by using an Integer Linear

Programming (ILP) approach to enhance the reconstruction accuracy of velocity models. This allows incorporating the sharp interface hypothesis directly into the reconstructed model. A Topology Optimization based ILP method is used to reconstruct a velocity model representative of the Santos Basina region, known for its thick salt layers. The ToS is assumed to be known, and an integer optimization variable is used to identify the salt region, the reservoir and the basement beneath it. Gradient filtering is used in order to control the appearance of spurious artifacts and to stabilize the inversion procedure. The influence of these filter parameters on the quality of the reconstruction is discussed.
The proposed approach showcased the capacity in locating and defining both salt bodies and hydrocarbon reservoirs. The exploration of the influence of the filters showed that the stabilization filter is fundamental for obtaining better results, and that the spatial filter, while effective in alleviating artifacts, may also harm the correct placement of material interfaces.

Keywords: Topology Optimization, Integer Linear Programming, Full Waveform Inversion, Salt model.

Introduction and Objectives: Understanding Earth's subsurface structures, particularly formations involving salt bodies, is essential for various geological and environmental applications. Salt bodies, formed through the deformation of evaporite salts over geological periods, lead to complex structures that influence hydrocarbon reservoirs, playing a pivotal role in hydrocarbon exploration. Full Waveform Inversion (FWI), a technique used to identify parameters in wave propagation systems, faces challenges in the presence of salt bodies due to their complex geometry and high impedance at sediment-salt interfaces. While approaches like level set methods and Total Variation (TV) regularization have been utilized to address these challenges, they hold inherent limitations such as being constrained by initial estimate topologies and introducing unwanted inversion artifacts, respectively. Topology optimization (TO) through Integer Linear Programming (ILP) is emerging as a viable alternative in handling sharp interfaces seen in geological formations with salt bodies. ILP in TO facilitates the representation of acoustic properties in these cases, since the interface contrast is assumed throughout the imaging process and offering, consequently offering a method that may lead to more accurate subsalt reconstruction.
The primary aim of this work is to develop and implement a procedure for inverse problems subject to wave propagation using Integer Programming to incorporate a-priori knowledge about the presence of sharp interfaces. The specific objectives are:
- Apply the multimaterial model from TO to subsalt reconstruction cases, focusing on the delineation of complex geological formations accurately. By introducing appropriate filters in TO, this work intends to mitigate the generation of spurious artifacts, aiming for improved delineation in seismic inversion processes.

Methodology: The wave equation is discretized in the time domain with a second-order explicit scheme. Spatial discretization is carried out through the Finite Element Method (FEM), employing triangular linear elements that result in a diagonal mass matrix. The implementation

leverages the Firedrake system, an automated solution for partial differential equations using FEM, and the Python package SPIRO, a wave propagator built on top of Firedrake. The IBM ILOG CPLEX Optimizer is used for the Mixed Integer Programming (MIP) problems in this work. The procedure consists in evaluating both forward and adjoint problems by using SPIRO, integrated with CPLEX for model updates. The optimization is bound by specified convergence thresholds and the material model used to link optimization variable and acoustic velocity.

Preliminary results: A multimaterial mapping was used to link the optimization variable to the acoustic velocity, initiating with horizontal layers of reservoir and basement materials as initial guess. A series of sweeping experiments were conducted to understand the influence of spatial (r) and stabilization (γ) filter parameters on the reconstruction. The analysis highlighted the significant role of the spatial filter parameter in maintaining a balance between artifact reduction and the accuracy in delineating the salt layer in the upper portions of the model. A qualitative analysis of the inversion results indicated that despite an apparent reduction of artifacts in configurations with $\gamma=0.9\gamma=0.9$ and $r=0.25r=0.25$, it did not necessarily yield the best agreement with the reference model. In fact, configurations within $0.05\leq r\leq 0.10.05\leq r\leq 0.1$ and $0.9\leq\gamma\leq 0.9990.9\leq\gamma\leq 0.999$ presented better reconstruction of the salt layer despite the presence of artifacts, thus illustrating the nuanced role of the spatial parameter r. In addressing the inverse crime issue, the addition of Gaussian noise to the reference signal was considered, and inversions were carried out under various filter parameter configurations. The insights derived indicated an augment of artifacts in the absence of inverse crime, especially noting the emergence of reservoir artifacts on the previously well-defined salt layer. Moreover, the study revealed that higher spatial filter weights could mitigate the noise impact, but that the same did not happen with variations in the stabilization filter weight.

Preliminary conclusions: Substalt reconstruction was successfully carried out. Initial results highlight the imperative of careful selection of spatial and stabilization filters parameters and a detailed approach towards inverse crime to obtain reliable velocity models. Further research is needed in order to strike a balance between accurate interface detection and artifact avoidance.

Icaro Amorim de Carvalho
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Abstract Title: Topology optimisation of a rotor subjected to a transient and compressible fluid flow

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Abstract: Unsteadiness is closely related with the vortex dynamics that leads to surge and stall phenomena in compressor rotors, which affect compressor's performance. Despite previous efforts, the literature still lacks a formulation in topology optimisation to evaluate turbulent, compressible fluid flows that are time-dependent, and thus motivates this study. We handle this class of problems. First, the optimisation will be assessed preliminarily in compressible and laminar regime, to consecutively advance on the matter of turbulence, with Favre-Averaged Navier-Stokes equations. Finite volume simulations will be carried out in OpenFOAM to resolve the fluid flow problem, while FEniCS will provide the automatic differentiation necessary to find relevant sensitivities of the problem. A combination of the two is found in the FEniCS TopOpt Foam framework (Alonso, Garcia Rodriguez, and Silva, 2021), which will be employed here. We specifically envision to optimise the design of compressors through this methodology to attenuate the formation of vortices and yet allow pressure gain, in a multiobjective function. This is justified in view of the gap in the literature of studies toward this goal. At present, literature review and preliminary simulations have been conducted.

Keywords: Topology optimisation. Computational Fluid Dynamics. Turbomachinery.

Introduction and Objectives: Global warming is amongst the major challenges of the century with dire consequences. In order to counteract CO2 -emissions to the atmosphere, Carbon Capture and Storage (CCS) and Utilisation (CCU) technologies offer viable means to contribute toward this goal. Beyond capturing CO2, CCU provides a means to transform carbon dioxide in material with product value. Technical processes in CCS converge to the compression stage, responsible for 50% of the performance of the entire CCS process (Rodriguez, 2022). Currently, the dissemination of CCS technology relies largely on the improvement of the compressor's performance. One-dimensional, parametric and shape optimisation are incapable of handling the extenuating number of parameters that are related to the operation of the compressor. To overcome these difficulties, topology optimisation is suggested here. It is a more generalist approach, independent of the initial design. A formulation to treat steady-state flow cases has already been developed and tested. Nevertheless, despite previous efforts, there is still no methodology to evaluate turbulent, compressible fluid flows that are time-dependent in topology optimisation. We intend to handle this class of problems. Unsteadiness is found in start-up, shutdown, and is related with the vortex dynamics that leads to surge and stall phenomena, which affect compressor's performance, and thus motivates this study. We principally envision to optimise the design of this turbomachine through the FEniCS TopOpt Foam framework (Alonso, Garcia Rodriguez, and Silva, 2021) with Favre-Averaged Navier-Stokes equations, employed with finite volume discretisation. Within the scope of non-rotating and rotating, compressible, turbulent, and time-dependent flows of Newtonian fluids, we intend to test previous penalisation procedures and adapt to transient simulations; incorporate the time transient aspect to the optimisation using the FEniCS TopOpt Foam, developed by Alonso, Garcia Rodriguez, and Silva (2021); develop and apply the methodology to time-transient cases related to the centrifugal compressor, in particular to avoid surge and stall and thus enlarge the range of operation of the compressor; and conduct other relevant time-dependent examples.

Methodology: This work intends to use two robust open-source software. OpenFOAM (finite-volume C++ "Open-source Field Operation And Manipulation", Weller et al., 1998; ESI, 2020) will be employed for the computations of the direct problem, that is, the simulation of the time-dependent compressible fluid flow; while FEniCS, combined with the dolfin-adjoint library will be devoted to the computation of the sensitivities of the problem through a finite element implementation for the computation of the discrete adjoint (Logg, Mardal, and Wells, 2012; Farrell et al., 2013; Mitusch, Funke, and Dokken, 2019). As such, OpenFOAM will be used to conduct finite volume simulations for compressible flow simulations with adequate choices of discretisation scheme (to be defined). Previous works converge that the use of the one-equation turbulence model of Wray and Agarwal (2015) provides good results (Alonso et al., 2022; Rodriguez, 2022). Communication between OpenFOAM and FEniCS will follow the structured methodology explored by Alonso, Garcia Rodriguez, and Silva (2021).

Preliminary results: At present, the author has advanced on the literature review and conducted preliminary compressible flow simulations with exemplary initial design to assess the time-dependent implementation in the FEniCS Top Opt Foam framework.

Preliminary conclusions: The author is still within the Preliminary part of the project.

Teresa Duarte Lanna
Institute of Physics, DFMT, University of Sao Paulo

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP) and sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by Petronas, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Li separation from production water using ZIF-67

Authors' Names & Affiliation Institutions of all authors (in order for publication): Institute of Physics, DFMT, University of Sao Paulo.

Abstract: The water (produced water - PW) produced from O&G exploration contains metals and pollutants, such as lithium and boron, which are thrilling elements from social, economic, and technological points of view. The management of PW has become an essential part of the feasibility of gas and oil industry development. This research used atomistic simulations such as molecular dynamics (MD) and Density Functional Theory (DFT) first-principles calculations

to develop a membrane based on nanostructured materials to separate and recover Li from PW efficiently. Combining these methodologies allows for the fundamental understanding of properties, including adsorption energies and molecular configurations. Using MD simulations, it was possible to characterise the transport and structural properties of ions present in the PW, using different compositions of each ion in bulk water. Calculations at the electronic level gave us the adsorption energies of the substances present in PW on the candidate materials for the separation process. We used DFT calculations to study the ZIF-67 electronic structure, which can be used as a nanofiltration membrane to separate Li from PW. We obtained the most favourable adsorption sites of Li in ZIF-67. The findings obtained in this work may serve as an essential guideline for designing and manufacturing nanostructured materials with unique properties for separating Li and B from PW.

Keywords: DFT calculations, ZIF-67, nanofiltration membrane, MD calculations, Lithium, produced water.

Introduction and Objectives: The water (PW) produced from O&G exploration contains large amounts of metals and pollutants, such as boron (B) and lithium (Li) [Ezechi et al., 2012]. Social and economic interests and technological challenges exist in developing methods for treating PW as a source of human and agricultural consumption [Igunnu & Chen, 2014]. Various techniques, including physical processes such as membrane filtration, can be used for the PW treatment.

This project aims to develop novel technologies based on nanotechnology and advanced materials for Lithium (Li) and Boron (B) separation from produced water (PW). One of the promising materials is metal-organic frameworks (MOFs), capable of filtering and recovering B and Li ions from PW. Here, atomistic simulations were used to investigate and characterise the PW and the transport and thermodynamics properties of a subclass of MOFs, the Zeolitic imidazolate structure (ZIF). ZIF systems exhibit mechanical flexibility and have received extensive research interest in this subject area [Zhong et al., 2018]. In particular, we focus on the ZIF-67 structure, which can be synthesised by a facile and environmentally friendly organic synthesis method and has characteristics of a tunable pore aperture ideal for filtration processes. To describe and characterise each ion separately, we studied the molecular model of the PW. The molecular model mimics PW in most studies because of the significant variance in PW composition. We executed simulations of the different ions isolated and in various combinations in water. We obtained structural, transport, and thermodynamic properties such as radial distribution function, diffusion coefficient, and density. This information was used to validate our force field choice and will be used as a reference to simulations composed of other mixtures of ions.

Methodology: DFT allows us to obtain the electron density and any physical observable, and it was employed using the Kohn Sham scheme, the plane-wave basis projector augmented wave method and optB86b-vdW [Klimes et al., 2011] exchange-correlation functional as implemented in the VASP package. DFT was used to calculate the adsorption energy of the

substances present in PW, such as Li, on ZIF-67. Adsorption energy property allows us to understand how the membrane interacts with a guest molecule once information on the strength of the adsorption energy determines if the adsorption happens through a physical or chemical process. To calculate the adsorption energy of Li at different adsorption sites, we insert a Li molecule near the site of interest and relax the atomic positions, minimising the total force in the atoms. Using the total energy of the system (pristine or thermally treated ZIF-67 + Li), we can determine the adsorption energies (Eads) involved and the electronic structure changes due to the interactions involved.

It is also important to describe correctly the behaviour of the isolated ions molecules to recover Li properly. We performed MD simulations using LAMMPS software to obtain the structural and transport properties of systems composed of the different PW ions, separately and in combinations. The radial distribution function [G(r)] is a structural property obtained from the average position of all atoms in the simulation; it presents how the material is structured and ordered in space and gives information about its physical phase. The diffusion coefficient is a transport property that helps us understand the dynamics of the guest PW molecules inside the ZIF. We use Einstein's equation, which relates the diffusion coefficient with the particles' mean square displacement (MSD). Since the simulation must be neutrally charged and Li+ is positively charged, we added a negatively charged ion, Cl- (contra ion), to neutralise the system. Different system concentrations were considered, and simulations were performed at 1 atm, with 300 and 350 K parameters to describe Cl- obtained from [Bonthuis, Mantkulov, and Netz, 2016], TIP4P was used to describe the water molecules and Li+ [Jaadasdasdasfadfasung and Cheatham III, 2008].

Preliminary results: Using MD, we studied molecular models of PW systems composed of bulk water with different compositions of the ions and obtained transport and structural properties such as self-diffusion coefficient, density and the G(r) of Li for water atoms. With those properties, it was possible to validate our force field models. Then, it provided information about the effect of different water compositions on the system's thermodynamic properties and ion structuration in PW. We will also use it to reference the following simulations of more complex systems composed of a mixture of molecules, as present in the PW molecular model. Since the hydration shell of ions and molecules plays an essential role in the separation processes, we determined the size of the first hydration shell of boric acid and lithium from G (r).

Preliminary conclusions: In this work, we performed MD simulations of Li+ and other PW ions in bulk water. With these simulations, we obtained structural and transport properties, such as radial distribution function, self-diffusion coefficient and density, that were compatible with the results presented in the literature. We also obtained the ions hydration shell since it is important information to select the best materials as membranes for Li separation. ZIF-67 was properly characterised at an electronic level using DFT calculations. We relaxed the structures and compared them with experimental lattice parameters while obtaining these materials' electronic properties. We calculated the interaction energy between these frameworks and the

ions of produced water and got the most favourable adsorption sites of Li in ZIF-67. The findings obtained through DFT and MD may serve as an essential guideline for designing and manufacturing nanostructured materials with unique properties for separating Li from PW.

SHORT ORAL SESSION F

14h - Short Oral Session F

0911 – EMS21 (TV1)

Chairs: Alberto Fossa – Maurício Salles

Andre Luis Ferreira Marques
University of São Paulo - USP

Abstract Title: Solar energy and GHG: a Data Science case study in the Manaus-Parintins Axle"

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Abstract: Renewable energy options have increased their weight in the energy transition actions taken worldwide. Solar energy has enlarged its presence in residences and dedicated farms, presenting an alternative energy source for fossil fuel thermal units, contributing to dim the GHG emissions. This renewable energy option can be used in rainforest environments, like the Amazon Basin, whose importance is highlighted in climate stability maintenance. However, to allow better life standards in those areas, solar energy prediction requires methods based on data, such as Artificial Neural Networks, to consider the natural intermittence and the influence of meteorological and environmental variables, such as the GHG. This research focused on applying Data Science frameworks to evaluate the use of solar energy incidence (W.h/m²) in the axle between Manaus and Parintins, both cities in the Amazonas state, considering open-source data from ground stations, monitoring towers and satellites. The research presents a visual distribution of solar energy and the cross-relation between local temperature, wind speed and CO2, allowing some conclusions on using the solar energy in the specific axle.

Keywords: Solar energy, GHG, Artificial Neural Networks, Amazon Basin, Data Visualization.

Introduction and Objectives: The changing environmental conditions in recent decades have emphasized the need for new technologies and innovations to handle the consequences of human activity. The quest for alternatives to fossil fuels has strengthened the role of renewable energies, such as wind, biomass, and solar power, in reducing the generation of greenhouse gasses (GHG), such as carbon dioxide and carbon monoxide (CO2 and CO), and meeting growing electric energy demand. Renewable options have augmented their share in the energy matrix of many countries. This research handles solar power prediction using Artificial Neural Networks (ANN) in the Amazon Basin because it is a free and flexible option. As engineering materials, power storage hardware, digital control technologies, and transmission lines continue

to develop, better solar systems have emerged within smart electric grids used locally. Forecasting solar power incidence is crucial for larger and floating systems in this effort. Solar panels are ideal for remote areas with limited energy supply alternatives compared to thermal electricity units burning fossil fuels, with a greener logistic chain. They are also easily installed on mobile units, like riverboats or small houses, to improve local living standards. Solar panels in the Amazon Basin, the world's largest rainforest, offer a low-impact energy generation that minimizes environmental harm. Therefore, the region is a prime candidate for adopting solar power, with the potential benefits of decreasing environmental impact (less local generation of GHG generation from thermal electric power stations), enhancing local living standards, promoting sustainable energy production, and decreasing the need for complex supply chains (e.g., gas pipelines or oil barrels). The region of interest is the axle between Manaus and Parintins. The time window of this research covers five years, from January 2018 to January 2023. The research aims to assess the influence of meteorological variables and GHG concentration (input variables) in the solar energy incidence (target variable), providing a visual distribution of the input and target variables, using ANN to predict the solar energy in the region above.

Methodology: The initial steps take data from open sources, such as the Instituto Nacional de Meteorologia (INMET), NASA satellites and monitoring towers. These data were aggregated daily. After a data health check and treatment, exploratory data analysis is carried out to provide a first set of insights about the relation between the input and target variables. The feature importance allowed us to understand how the input variables may explain the solar irradiance in the region and hinted at the priority of the variable selection for the ANN development. From this EDA, the first data visualizations are made available. With data ready, the ANN was developed, here a Long Short-Term Memory with a Gate Recurrent Unit (LSTM-GRU). The prediction time horizon was three days ahead, linked to energy system management, such as electric batteries. The performance metrics used were the Mean Absolute Percentual Error (MAPE) and the Root Mean Squared Error (RMSE), which were compared to other similar references.

Preliminary results: Tables and figures about the application of the methodology above showed the influence of the weather variables in solar incidence, considering the forecast time of three days.

Preliminary conclusions: The relations among the input variables, mainly the GHG and local temperature, show a clear impact on the solar irradiance in the region.

João Fegadolli Nunes da Silva
EACH-USP* IEE-USP*

Abstract Title: Assessment of Biomethane Potential for Urban Agriculture

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Thiago Luis
Felipe Brito
Dalmo S Amorim Jr
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Abstract: This study aims to enhance the understanding regarding the feasibility of implementing an urban waste biodigester in small clusters by conducting a literature review and systematic analysis to evaluate the potential for energy generation within a specific locality.

Keywords: survival, land, waste, biodigester, biogas.

Introduction and Objectives: Urban survival requires political, technological, and community interventions to meet the collective needs demanded by social coexistence within the spaces provided by cities. Therefore, even minimal assistance in mitigating basic costs can lead to improvements in the quality of life for the population in large metropolitan areas. Urban agriculture presents an alternative means to reconnect humans with the land, addressing a primary source of food, medicinal and ornamental plants. It can be implemented in available spaces such as municipal parks, squares, gardens, lots, rooftops, yards, schools, health centres, central medians, and wherever innovation and utilization can lead. Through the application of agroecological management techniques, it becomes possible to optimize crop yields. One such technique is the implementation of a biodigester, which, similar to the encouragement of new energy cycles throughout millennia, has allowed various types of biomasses to supply a significant portion of society's energy needs, transitioning in recent decades between coal and petroleum. However, the use of natural gas derived from petroleum has raised growing concerns about environmental degradation, prompting societal actions to enable renewable sources Given the importance of urban farming, it is expected that agricultural production residues will be generated through management and pruning. These residues undergo decomposition, releasing their nutrients through the emission of methane (CH4) and carbon dioxide (CO2), primarily forming biogas. These gases can be captured through a biodigester, which stores gas and organic matter anaerobically. The digestion of the material is facilitated by microorganisms sustained by the constant supply of organic compounds. Additionally, nutrients contained in the biomass that are not converted into gas by bacteria are returned as ready-to-use organic

fertilizers for cultivation. The resulting product can contribute to generating extra income while minimizing environmental impacts through organic recycling, providing economic benefits to those willing to utilize it. Thus, the use of biogas aligns with addressing the issues presented. As a sustainable and renewable alternative in the short term, this study assesses the feasibility and effects of implementing a food waste biodigester in small agroecological clusters.

Methodology: In Brazil, an average of 1.2 kilograms of organic waste per inhabitant is produced daily, often without proper disposal. Such waste can be redirected for energy production instead of being disposed of in landfills and dumps, which are the primary sources of methane emissions. It is estimated that the treatment and disposal of urban waste account for 13% of total anthropogenic greenhouse gas emissions. Taking this issue into consideration, the Urban Farm, the initial case study of this research, is an organic urban garden located in the southern region of the State of São Paulo in the Ipiranga neighbourhood. It promotes and encourages the disruption of traditional cultivation models through techniques aimed at maximizing scarce resources within the city, re-establishing people's connection with the source of their food, and seeking to preserve and value cultural habits. The Urban Farm project is partly supported by the Hortas em Rede initiative, a collaboration between the National Electricity Entity. Its central goal is to transform ENEL's spaces into productive and sustainable areas, enhancing the effective management of easements and promoting local socio-economic development. A composting zone was established on this site. Due to a shortage of waste resulting from the type of cultivation, a collaborative effort was organized involving the municipality, school, market, businesses, and residents of the neighbourhood to dispose of pruning and food waste.
In this way, the researcher engages in a dialogue with the organization to assess potential forms of training and implementation, involving professionals in the field, active composting, and improper waste disposal, evaluating the capacity for production in unique community systems.

Preliminary results: Currently, the urban garden in question has a total area of 1300 m³, producing an average of 680 kilograms per month using agroecological methods. As it primarily focuses on vegetables, approximately 80 kilograms of productive waste are acquired each month, which is directed to a small scale vermiculture system. The composting facility collects an average of 10 tons of organic matter per month, equivalent to 30,000 m³ of biogas. This biogas can be utilized for cooking or converted into electrical energy.
Based on this data, it is possible to estimate the customized size of the biodigester based on the volume of organic matter. The best type of biodigester will be designed, considering costs and maintenance, to achieve the benefits of biogas production.

Preliminary conclusions: This study aims to generate knowledge regarding the requirements for the small-scale implementation of organic matter biodigesters for biogas production, guided by a case study. Additionally, it intends to identify communities in the eastern region of São Paulo with potential for waste generation and storage for biogas production, pinpointing

locations that produce viable types and quantities of waste and possess the necessary physical space for biodigester construction.

Letícia Souza de Jesus

Enhancing Predictive Maintenance and Diagnostic Techniques for Stator Fault Detection Using Mathematical Models and Python Simulations

We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation (23.1.8493.1.9), hosted by the University of São Paulo (USP), sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5), and sponsored by TotalEnergies, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

Abstract Title: Enhancing Predictive Maintenance and Diagnostic Techniques for Stator Fault Detection Using Mathematical Models and Python Simulations

Authors' Names & Affiliation Institutions of all authors: Letícia Souza de Jesus (Affiliation: University of São Paulo) and Maurício Barbosa de Camargo Salles (Affiliation: University of São Paulo).

Abstract: The present project aims to improve predictive maintenance and diagnostic techniques, monitor the winding condition, and detect stator fault trends. In this way, tools are proposed to monitor the winding condition and detect stator failure trends using mathematical models and computer simulations in Python, in order to avoid the need for additional sensor installation, and with the mathematical description, it is possible to understand the impact of these faults and support the interpretation of experimental results. Defects between stator windings cause specific changes in the harmonic content of generator line and field currents, which are filtered and used for detecting them. Selected harmonic components at different speeds, dynamic filters based on *abc/dq* and Fourier transforms are used, which employ rotor position measurement to adapt to changes in frequency components under different speeds. Then, geometric locations are proposed as parameters to distinguish between healthy and faulty conditions. To this end, a Python code will be proposed to simulate its operation under the effects of these faults.
Keywords: three-level; internal faults; external faults.

Introduction and Objectives: The contribution of wind generation in Brazil is expected to grow further in the coming decades with the construction of offshore wind farms, which will be used to decarbonize oil and gas extraction processes, and also integrated into the National

Interconnected System (SIN). Therefore, growth in this type of generation is expected, with the installation of more variable speed generators. As the contribution of variable speed generators to the SIN increases, greater attention must be paid to the maintenance and protection aspects of the equipment and greater efforts must be made to keep them operating optimally. These generators are subjected to adverse conditions and are subject to mechanical or electrical failures. Among these defects, turn faults stand out which, depending on the distribution of the stator windings, may involve turns of the same phase or different phases and are divided into the types of faults reported in the literature: Between Turns (EE), Between Branches (ER) and Between Phases (EF), which may or may not involve the Earth [1]. If not detected in advance, these faults can damage the entire generator winding.
Aiming to corroborate these predictive maintenance and diagnostic techniques, monitor the condition of the winding and detect the failure trend, the research project seeks to simulate the operation of the synchronous electric generator under fault conditions, through the collection of differential equations and implementation with codes in Python.
[1] MONARO, R. M. H. et al. Experimental platform for controlled faults on synchronous generator armature windings.
IEEE Transactions on Energy Conversion, IEEE, v. 27, n. 4, p. 948–957, 2012. ISSN 08858969.

Methodology: The methodology of this project comprises a detailed analysis of the effects of faults in the synchronous generator, focusing on faults in the stator winding, using mathematical equations implemented in Python, with the aim of understanding the effects of these faults and supporting the interpretation of experimental results.

Preliminary results: Project still in progress, so there are no results yet.

Preliminary conclusions: Project still in its initial phase, so no conclusions at the moment.

Stevan Henrique Ramon de Góes
UFSCar

Abstract Title: Using Artificial Intelligence for Image Analysis in Monitoring the Condition of Wind Generator Blades

Authors' Names & Affiliation Institutions of all authors (in order for publication): stevanrrgoes@gmail.com

Abstract: Predicting and detecting damage to wind turbine blades involves an extremely important role in optimizing wind energy generation operations. This capability not only contributes to ensuring the structural integrity of the turbines, but also plays a crucial role in

preventing the need for corrective maintenance caused by unforeseen failures. The ability to anticipate and identify damage at an early stage enables the implementation of programmed and targeted interventions, avoiding unexpected interruptions in production and considerably reducing the costs and resources associated with reactive maintenance. Therefore, effective prediction of damage to wind turbine blades not only preserves operational reliability, but also has a significant impact on resource savings, improving the overall efficiency of wind generation facilities.

Keywords: detecting, damage, prediction, wind turbine blades, optimizing.

Introduction and Objectives: This research work explores the importance of wind turbines, aiming to build a technological energy scenario through the incorporation of Deep Learning techniques to significantly contribute to the mitigation of unforeseen maintenance. Deep Learning is an approach to machine learning that is based on the construction of computational models composed of multiple layers of processing, seeking to capture hierarchical and abstract representations of data. Central to this approach are Artificial Neural Networks, mathematical structures composed of interconnected nodes, which seek to emulate the functioning of biological neurons. These networks consist of successive layers, where each layer processes and transforms the input signals before transmitting them to the next layer. By applying optimization algorithms and adjusting the weights of connections between nodes, neural networks can learn to identify complex patterns in data, allowing tasks such as pattern recognition, classification and anomaly detection with a high degree of accuracy. In the contemporary scenario, where digitalization and automation play a central role in almost all aspects of life, the early detection of anomalies and failures plays a critical role in maintaining the integrity of complex systems. Deep learning, being a subarea of artificial intelligence that emulates the functioning of the human brain, has emerged as a powerful tool for identifying subtle and non-trivial patterns, often imperceptible to traditional analysis methods. This research work addresses the relevance of deep learning in detecting anomalies in wind turbines, exploring its theoretical bases and practical applications. By uncovering the ability of this approach to improve the accuracy and efficiency of damage identification, this article aims for transformative potential in the field of wind turbine blade maintenance. The accelerated expansion of wind energy as a sustainable energy source has highlighted the importance of ensuring the reliability and operational efficiency of wind turbine systems. Damage to wind turbine blades, resulting from factors such as environmental stress and wear over time, presents considerable challenges to the sustainable operation of these systems. The ability to accurately predict, detect and segment this damage is crucial, not only to avoid unforeseen interruptions, but also to optimize the allocation of resources for maintenance. This academic work introduces an interdisciplinary exploration that encompasses advanced deep learning techniques, image analysis and unmanned aerial vehicles (UAVs) responsible for capturing data. Based on these different studies, the article contemplates the integration of these methodologies to improve the identification and classification of damage to wind turbine blades.

Methodology: The methodological approach of this article consists of proposing a Neural Network model for segmenting images of wind turbine blades. The model is trained and tested on a dataset of images captured and provided from a wind farm by through drones. Before training, the images are manually annotated at the pixel level and converted to grayscale, the pixel values representing the background and the turbine blade, respectively. The data set consists of a bank of images of wind turbine blades, and were separated into training, having their masks labeled, and test, comprising 35% of the total images provided. To improve segmentation accuracy and reduce computational complexity, the Neural Network (U-Net) model uses depth-wise separable convolution and fusion of batch convolution and normalization layers. Furthermore, the model employs a residual neural network (ResNet) as a backbone for feature extraction and attention mechanisms to capture important details in images. Experimental results show that the improved U-Net outperforms other segmentation methods in terms of average intersection over union and average pixel accuracy. Furthermore, the model has a faster execution time compared to other models.

Preliminary results: Project still in progress, so there are no results yet.

Preliminary conclusions: Project still in its initial phase, so no conclusions at the moment.

0911 – BECCUS13 (TV2)

Chairs: André Dourado – Marcos Buckeridge

Thiago Vasconcelos de Barros Ferraz
São Carlos Institute of Chemistry - IQSC

Abstract Title: Enabling ethanol electro-oxidation in seawater-like electrolytes for energy conversion and CO2 mitigation

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Abstract: The global temperature increases and alarming climate occurrences led 195 nations to sign the Paris Climate Agreement in 2015, committing to limit global warming to 1.5 °C - 2 °C by 2100. Achieving this goal requires fast decarbonization of key productive sectors by 2050 and subsequent active removal of 10-20 Gt of atmospheric CO2 annually. Among the existing mitigation alternatives, a promising one involves adapting the rapidly expanding desalination infrastructure worldwide for the parallel electrochemical capture and mineralization of CO2

into chemically stable CaCO3 and MgCO3 salts - which can be safely stored in the seafloor for hundreds to thousands of years. Many thermodynamic/technic constraints associated with the use of the of hydrogen oxidation (HOR, E° = 0 V vs. RHE) or oxygen evolution reactions (OER, E° = 1.23 V vs. RHE) as half-cell anodic reactions in support systems for such application have been overcome with some success in the field of fuel cells by replacing them with the oxidation of biomass-based low molecular weight aliphatic alcohols – which tend to exhibit comparatively modest thermodynamic oxidation potentials (<0.5 V vs. RHE). Nonetheless, the Cl- anions in seawater (~0.56 M) are already well-known to cause the poisoning of transition metal-derived electrodes for organic compound oxidation, even in trace amounts at acid and neutral pH conditions. Herein we report on the seawater-like electrolytes alkalization as a way to enhance the feasibility of ethanol oxidation in such naturally chlorine-rich media. Polycrystalline platinum was chosen as model catalyst to be used in a three-electrode cell and an ethanol concentration of 1 M was maintained throughout the measurements. The potentiodynamic polarization tests indicated an enhancement in the current densities of the ethanol anodic processes with increasing pH values - consistent with a decrease in the specific adsorption strength of the Cl- anions on the Pt surface - reaching up to 3 mA cm-2 at 0.69 V (vs. RHE) in a solution with a non-depleted chloride level of 0.5 M and pH of 14. Furthermore, the aforementioned adjustment of the experimental parameters allowed us to access dynamic instabilities in the form of potential oscillations – which otherwise do not appear in the purely representative environmental near-neutral pH of 8.2 - and that can be, in principle, harnessed to improve the power density delivered by electrochemical devices operating under the proposed conditions.

Keywords: Electrocatalysis, Seawater, Ethanol Electro-oxidation, Dynamic Instabilities.

Introduction and Objectives: The noticeable increase of the average global temperature in recent decades – and the coincident occurrence of alarming climate events – led in 2015 to 197 nations to sign the Paris Accord, in which they committed to take part in a joint effort to limit the global warming to 1.5 °C – 2 °C (above the pre industrial levels) by 2100. However, in order for this goal to be achieved, not only a fast decarbonization of the key productive sectors of the economy is required to happen by 2050; around 10 – 20 Gt of atmospheric CO2 will also need to be actively removed and safely immobilized every year from that point forward. Among the various groups of alternatives under evaluation (e.g., DAC and BECCUS), those proposing the use of the oceans – the largest natural carbon sink known – are receiving growing attention since they are the only ones capable of tackling the scale of the challenge. One of the most promising involves adapting the rapidly expanding desalinization infrastructure around the world with parallel electrochemical processes able to capture the CO2 and mineralize it in the form of chemically stable CaCO3 and MgCO3 salts – which can be harmlessly stored in the seafloor during hundreds to thousands of years. A major conceptual energy limitation of the previous approach resides in the intrinsic overpotentials required for the electrochemical device to operate with significant current densities. Usually, water oxidation or hydrogen oxidation are applied as the anodic half-cell reaction on such devices, though the former suffers from the lack

of efficient, stable and commercially available catalysts, and the gas diffusion anodes required by the latter are still on the course of being adequately scaled up. Such difficulty has been circumvented with a good degree of success in the field of fuel-cells by replacing the oxygen evolution reaction (OER, E° = 1.23 V vs. RHE) and the hydrogen evolution reaction (HER , E° = 0 V vs. RHE) with the oxidation of biomass-based low molecular weight aliphatic alcohols (e.g., methanol, ethanol, glycerol) – which tend to exhibit comparatively modest thermodynamic oxidation potentials (~0.10 V vs. RHE). Nonetheless, an important aspect to consider is that seawater possesses extremely high Cl- concentration (around 0.56 M), which has been long well reported to poison the surface of most transition metal-derived electrodes to organic compounds oxidation in general, even in trace amounts in acidic and neutral media. In light of the exposed, in this work, we approached the alkalinization of seawater-like electrolytes as means of increasing the energetic and economic feasibility of applying the ethanol oxidation reaction (EOR) in such naturally chlorine-rich medium.

Methodology: The experiments based on voltammetry, electrochemical impedance spectroscopy, and galvanostatic and galvanodynamic assays were carried out following procedures previously described in the Group's previous works. In all cases, a single-compartment electrolytic cell using a three-electrode configuration was employed. A flat polycrystalline platinum electrode of 5x5 mm was set as the working electrode, while a high-surface-area platinum spiral was adopted as the counter electrode, and a reversible hydrogen electrode (RHE, with double junction in the case of measurements conducted at pH > 2 and < 12) served as the reference electrode. All solutions were prepared using analytical-grade reagents in high-purity water (Milli-Q, 18.2 MΩ cm). The measurements were performed using a potentiostat/galvanostat (model PGSTAT302N) from Autolab®, equipped with the manufacturer's Nova® interface, which served for both system control and data preprocessing. Before each experiment, both platinum electrodes were briefly heated to incandescence with a butane/air flame and then inserted into the argon-purged system, with the temperature maintained at 25 °C using a thermostat bath. The electrochemically active area of the polycrystalline platinum electrode was determined before each experiment - for normalization purposes - by integrating the charge from the hydrogen desorption region in voltammograms obtained for a 0.5 M H2SO4 solution at 50 mV s-1 and between 0.05 V and 1.2 V. The ionic compositions of the solutions used in the experiments were primarily based on the values provided by the international standard ASTM D1141-98 for preparing artificial seawater, in which components present in concentrations < 1 mMol kg-1 were here disregarded for simplicity. In each set of measurements, the ionic strength of the anionic components was kept constant by adding appropriate amounts of HClO4 or NaClO4 to ensure better control over any observed trends. Finally, ethanol was chosen as the organic compound of focus due to its simpler structural properties compared to other aliphatic alcohols. Additionally, its concentration in the electrolyte solutions of interest was limited to 1 M due to the low solubility of magnesium and calcium hydroxides and (bi)carbonates present in the medium at higher concentrations.

Preliminary results: In the presented investigation, a series of experiments was conducted to explore the electrochemical behaviour of platinum electrodes in the presence of ethanol-containing solutions with varying pH levels - and with an ionic composition resembling that found in seawater environments. Initially, it was observed that the oxidation of ethanol in the presence of chloride ions, typically encountered in seawater, is fundamentally impractical without prior removal of chloride ions. However, as the pH of the solution becomes more alkaline, distinct changes in the electrochemical profiles become apparent. Between pH 10 and extending through pH 12, there is a notable intensification and splitting of the main peaks associated with the formation and reduction of platinum oxide. This phenomenon appears to diminish as the pH approaches 14. Similarly, the peak associated with hydrogen adsorption on platinum (110) also undergoes a slight splitting at pH 10, with a subsequent decrease as pH approaches 14. The exact reasons for these pH-dependent effects remain under investigation, with our main hypotheses suggesting a complex interplay between pH and the rates of underlying surface processes. Furthermore, in the solutions containing 1 M ethanol, a significant increase in current density was observed as the pH increased from 10 to 12. This indicated a relaxation of the inhibitory effect of chloride ions on the adsorption of organic molecules as the pH levels became more alkaline. Additionally, a phenomenon of peak splitting in the oxidation of ethanol on the electrode surface was observed at pH 12. This splitting suggests the accumulation of ethanol-derived species with shorter lifetimes, which diminish as the pH approaches 14. Moreover, since dynamic periodic instabilities could potentially be harnessed to reduce the theoretical energy consumption in electrochemical devices that oxidize organic compounds, Preliminary experiments in this regard were carried out in the standard system at pH 8 but did not reveal any indications of current windows where such desired potential oscillations could be observed. However, a comprehensive series of tests across a broad pH range indicated not only the appearance but also a reduction in the average period of oscillations and an increase in the number of oscillations as pH increased. This trend suggests an enhancement in the catalyst's reactivity for ethanol oxidation, facilitated by improved surface self-cleaning in response to adsorbed poisoning species.

Preliminary conclusions: The results obtained indicate the fundamental infeasibility of oxidizing ethanol under the natural conditions in which seawater is found in the environment unless it undergoes beforehand a thorough secondary process of removal of the chloride ion. However, there is still the possibility of harnessing the increasing in the medium’s pH to reduce the specific adsorption of the Cl- anions on the electrode surface - thereby allowing appreciable current density values to be attained from the alcohol oxidation at potentials lower than those who would be required for water or chloride oxidation reactions. This not only reopens but also expands the range of applications possible for the system of interest as an aid for atmospheric CO2 capture and mineralization efforts. For instance, the flow of alkalized seawater into the organic compound oxidation system could be provided by the catholyte of an electrolyzer feed with a saline solution directly extracted from the ocean or discharged by a desalination facility. Such an approach can increase both the amount of H2 generated per liter of solution used and reduce the long-term implementation costs of these processes through the commercialization of

higher-value products obtained from the incomplete oxidation of ethanol.

Paula Barione Perroni
USP/IQSC

Abstract Title: Stainless Steel as Catalyst for Ethanol Oxidation Reaction

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Abstract: This work investigated the viability of utilizing an austenitic stainless steel as an electrochemical catalyst for ethanol oxidation reaction (EOR), specifically the AISI310, which is rich in Ni. The catalytic activity for ethanol oxidation was examined using cyclic voltammetry. The reaction displayed sensitivity to the presence of various cations in the solution, indicating the influence of the size and intercalation of the ions in the superficial film of the Ni-containing electrode. The study also explored potential oscillations through galvanostatic experiments, revealing similar patterns with differences in frequency and potential window depending on the type of cation present. A Preliminary proposed mechanism for these oscillations suggests that NiOOH species are consumed during ethanol oxidation, limiting their availability for continued reaction by decreasing active sites and subsequent converting to Ni(OH)2. In summary, this study demonstrated that stainless steel electrodes have potential for ethanol oxidation and exhibit interesting catalytic characteristics. Nevertheless, questions persist regarding the influence of cations, indicating the necessity for future investigations to achieve a more comprehensive understanding of the electrochemical system under study.

Keywords: stainless steel, ethanol oxidation, nickel oxyhydroxide, oscillations.

Introduction and Objectives: Small organic molecules, particularly ethanol, show promise potential as power source due to its high hydrogen density, non-toxicity, ease of handling, and sustainable sourcing from biomass. Additionally, the CO2 produced during ethanol oxidation is part of the natural carbon cycle, originating from previously absorbed plant CO2. Employing noble metals as catalysts is not economically feasible due to their scarcity and high cost. Finding

a non-noble metal at lower cost is essential for the large-scale application of these energy sources. Stainless-steel contains elements favourable for electrocatalysis such as Ni and Fe, elements with potential as catalyst for both oxygen evolution reaction (OER) and ethanol oxidation OER. The introduction of Fe into NiOOH structures has been shown to significantly enhance catalyst activity for both of these reactions. Given the relevant purpose of developing non-noble catalysts, this work aims to use the advantages of stainless-steel composition as a catalyst for ethanol oxidation, contributing to the development of non-noble catalysts for sustainable hydrogen production.

Methodology: We selected a stem of the alloy SS310, which contains ~20% of nickel (related to Fe) and before the experiments, it was polished from 600 to 4000 water sandpaper, and cleaned with acetone in ultrasonic bath. A carefully electrochemical procedure was necessary to activate the electrode. A reversible hydrogen electrode (RHE) was applied as reference electrode and a platinum grid electrode as counter electrode. The reaction was studied in three different media: LiOH, NaOH and KOH, all of them at 1 M concentration, and ethanol oxidation was studied at 0.5 M. All the current density are corrected by geometric area of 0.44 ± 0.02 cm-2. The cyclic voltammetry was performed between 0.8 and 1.55 V(ERH) at scan rate of 50 mV s-1.

Preliminary results: The cyclic voltammetry highlights the activity of the SS310 to oxidate ethanol and its sensitivity to the electrolyte. It exhibits two anodic peaks associated with ethanol oxidation and one cathodic peak corresponding to the Ni2+/Ni3+ redox reaction. The activity with different cations follows this trend: KOH ≥ NaOH > LiOH, the same trend reported for another NiFe-based electrodes. We attribute this behavior to the intercalation of cations within the nickel layers and their relationship with the hydrated radii of the cations. Notably, potential oscillations were observed in all the electrolytes within the range of 1.45 and 1.57 V(RHE), corresponding to the conversion of β-NiFeOOH and γ-NiFeOOH, in a stable pattern. The potential window achieved for each cation becomes more evident when examining the derivative curve of potential over time as a function of the potential, highlighting the differences in each situation. In the presence of Li+ and K+ cations, they exhibit similar values regarding the rate of potential increase, ranging from 0.26 to 0.33 V s-1, as well as for the rate of decrease, which ranges from -0.56 to -0.85 V s-1. In contrast, the velocities observed with Na+ are notably smaller, varying between 0.15 and -0.33 V s-1. A possible mechanism involves ethanol oxidation occurring during the redox conversion NiFe(OH)2/NiFeOOH, with the oscillations happening on the potential window where this redox reaction takes place, influenced by the presence of cations.

Preliminary conclusions: This study introduces a new perspective on the utilization of stainless-steel in electrocatalysis as an effective catalyst for the oxidation of organic molecules. Stainless-steel exhibits potential as a relatively inexpensive catalyst for ethanol electrooxidation with a good electrochemical response. Furthermore, we observed sensitivity of the reaction to

the cation present in solution, which might be related to the size of the ions and insertion between the layers of Ni-Fe in the electrode.

Naiza Vilas Bôas
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Abstract Title: The electro-oxidation of ethanol under oscillatory regime on platinum-tin electrodes

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Abstract: The electro-oxidation of ethanol under oscillatory regime on platinum-tin electrodes The electrocatalytic oxidation of small organic molecules is of general importance for energy-related issues such as the fuel cells and electrochemical reform. The characteristics that emerge along the catalytic oxidation of small organic molecules critically depend on the coverage and nature of absorbates [1-3]. The common emergence of current and potential oscillations in these reactions is closely related to the reaction mechanism and implies the overall conversion, and thus on the performance of practical devices [4]. In the present work we study the dynamics of electrochemical oxidation of ethanol under oscillatory regime using tin-modified platinum electrode. Experiments were performed in a classical three electrode cell, polycrystalline platinum flags were used as working electrodes (WE), a graphite stick was served as counter electrode, and a reversible hydrogen electrode (RHE) was used as reference electrode. The investigation was focused on the role played by surface free sites and the presence of a step with a short-lived specie adsorbed at the electrode surface. To reduce the coverage of poisoning species, and thus to increase the main reaction pathway, chronoamperometry in platinum oxide region followed by potential sweeps or the adsorption of ad atoms, like tin, tin-modified platinum electrodes were used to assess the decrease in coverage of poisonous species. The experimental part includes protocols to invest control the effect of surface
coverage using chronoamperometry and cyclic voltammetry, as well as studies under oscillatory regime. The results show that the efficiency of ethanol electro-oxidation is preferred powered, on a less poisoned electrode surface, which is obtained through a self-cleaning process driven by the oscillatory electro-oxidation. These results are rationalized in terms of reaction mechanisms on both platinum and platinum-modified systems.

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Keywords: Electrocatalytic, scillatory regime, ethanol.

Introduction and Objectives: The electrocatalytic oxidation of small organic molecules is of general importance for energy-related issues such as the fuel cells and electrochemical reform. The characteristics that emerge along the catalytic oxidation of small organic molecules critically depend on the coverage and nature of absorbates. The common emergence of current and potential oscillations in these reactions is closely related to the reaction mechanism and implies the overall conversion, and thus on the performance of practical devices. In the present work we study the dynamics of electrochemical oxidation of ethanol under oscillatory regime using tin-modified platinum electrode.

Methodology: Experiments were performed in a classical three electrode cell, polycrystalline platinum flags were used as working electrodes (WE), a graphite stick was served as counter electrode, and a reversible hydrogen electrode (RHE) was used as reference electrode. The experimental part includes protocols to invest control the effect of surface coverage using chronoamperometry and cyclic voltammetry, as well as studies under oscillatory regime.

Preliminary results: The results show that the efficiency of ethanol electro-oxidation is preferred powered, on a less poisoned electrode surface, which is obtained through a self-cleaning process driven by the oscillatory electro-oxidation.

Preliminary conclusions: The oscillatory electro-oxidation reaction of ethanol with the ordered intermediates of platinum and tin considerably affects the oscillatory dynamics, compared to the reaction at an unmodified platinum electrode. Overall, the results show a substantial increase in catalytic activity on platinum and platinum tin surfaces for the electro-oxidation of ethanol. These results are rationalized in terms of reaction mechanisms.

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Abstract Title: Study of Ethanol Electrooxidation in Oscillatory Regime for Gaining Mechanistic Insights.

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Abstract: Ethanol is a candidate molecule to be used as fuel in the so-called Direct Liquid Fuel

Cells – DLFC's, but due to his sluggish kinetics of electro-oxidation and demanding of noble metals catalysts the practical usage in large scale is yet restricted. The complete ethanol electro-oxidation reaction (EEOR) can produce 12 electrons, but parallel routes lead to the formation of other byproducts, mainly acetaldehyde and acetic acid, in which only 2 and 4 electrons are extracted in the process respectively, lowering the efficiency. Despite many years of studies, the EEOR mechanism still not fully comprehended, so to shed some light and gather more information about the reaction mechanism, we are combining experimental studies in oscillatory regime with computational simulations of microkinetic modelling. Understanding how the EEOR proceeds can help in the rational design of catalysts and optimization of conditions to be used in fuel cells. In the presentation will be shown how we can use the complex dynamics of oscillatory regime to gain insights about the mechanism of ethanol electro-oxidation along with microkinetic modelling.

Keywords: Ethanol; electro-oxidation; reaction mechanism; modelling.

Introduction and Objectives: Kinetic instabilities and non-linear dynamics are common phenomena in the electro-oxidation of many small organic molecules, including ethanol. By applying the right conditions, we can observe oscillations of current and potential that can show mechanistic information that otherwise could not be seen with conventional technics. In oscillatory regime, reactions can be sort of "decoupled", so we can have a better understanding of the interaction between different intermediate species adsorbed in the catalyst surface. The main goal of the experimental investigation is to gain insights about how ethanol electrooxidation reaction proceeds and use this in microkinetic modelling to validate a mechanistic proposal.

Methodology: The experiments were conducted in a conventional three electrodes glass cell, with both working (WE) and counter electrode (CE) made of polycrystalline platinum. The electrolyte consisted of a solution of 0.5 mol L-1 of H2SO4. All potentials were measured against a reversible hydrogen electrode (RHE) made of the same solution of the electrolyte. The cell was constantly purged with argon. A potenstiostat/galvanostat Autolab PGSTAT302N was used for measurements. The ethanol concentration was varied from 0.05 to 1.0 mol L-1, and cyclic voltammetry and chronopotentiometry were recorded for all concentrations.

Preliminary results: The frequency, amplitude, waveform, duration, and potential drift of the oscillations in galvanostatic mode are highly affected by ethanol's concentration. This could be related to the products selectivity. In lower concentrations the route that produces acetic acid is

dominant, and acetate can adsorb and block active sites. In higher concentrations the route that produces acetaldehyde is dominant and the oscillations last longer.

Preliminary conclusions: The information gained in the study of ethanol electrooxidation in oscillatory regime are being used in microkinetic modelling simulations and can help to validate the mechanistic proposal. The knowledge of how the reactions proceeds at a surface level can be used for rational catalysts design and improvement of Direct-Ethanol Fuel Cells efficiency.

Marilin Mariano dos Santos
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Abstract Title: Perspectives of BECCUS technologies in Brazilian sugarcane sector

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Abstract: This study analyses the implementation of Bioenergy with Carbon Capture and Storage (BECCS) systems in ethanol production plants. Brazil is the world's largest producer of sugarcane and, therefore, has a great potential for coupling biofuel production with carbon capture and storage. The 2022/23 harvest reached more than 610 million tons of cane, which illustrate the magnitude of the sector, producing 37 million tons of sugar and 28.4 billion of liters of ethanol. The sugar and ethanol production process results in the production of large amounts of waste such as sugarcane bagasse, filter cake and vinasse, besides a huge energy and carbon capture potential by the large quantities generated. Thus, by implementing the BECCS technologies, Brazil has enough conditions to contribute to reduce global carbon emissions and to occupy a top position worldwide. In the specific case of the sugar and ethanol sector, CO2 generation and capture take place from bagasse burning and fermentation processes. Although, with the use of vinasse and filter cake for biogas production, the CO2 resulting from biogas purification to produce biomethane or also electricity production through the burning of biogas can also be captured. To illustrate the importance of implementing BEECS in the sugar-energy sector, a case study was carried out considering a medium-sized mill, whose installed sugarcane mill capacity is 1.6 million tons per harvest. This sugarcane process produced 13.7 million liters of ethanol, which results in the generation of 47,624 tons of filter cake and 1.58 billion liters of vinasse and 444,492 tons of sugarcane bagasse. With these scenarios the technical potential for

capturing CO2 per harvest is 734,444 tons, considering the use of biogas to generate electricity. From this total, 13% are from the fermentation process, 80% from sugarcane bagasse burning and 7% from biogas combustion to generate electricity. Taking into account the use of biogas for biomethane production, the estimated technical potential for capturing CO2 is 708,626 tons per harvest, 14.1% from fermentation process, 82.9% from the burning of bagasse and 3% from biogas purification. It is important to consider that the capture point with the highest amounts of CO2 results from bagasse burning, corresponding to the lowest concentration of CO2 (7 to 14% v/v). This results in a high-energy penalty and high capture cost due to the large volumes to be treated and the low concentration of CO2. Studies show that the energy penalty for capturing post-combustion CO2 can be between 15 and 20%. Thus, despite the technologies used to capture CO2, being commercial (TRL is 8 or 9) additional efforts are needed to reduce the energy penalty and, consequently, the cost of post-regulation capture. For the fermentation process due to the high concentration of CO2 (> 95%) and the low -energy penalty (approximately 6%), it is highly recommended for use in other processes or geological storage.

Keywords: sugar-energy sector; carbon capture; BECCS.

Introduction and Objectives: Since the Industrial Revolution, for centuries, fossil fuel consumption have resulted in significant environmental impacts, which is reflected in climate change worldwide. Together with the energy transition to use renewables replacing fossil fuels, carbon capture storage (CCS) is considered as one of the most promising technologies to reduce carbon emissions and avoid such emissions to be released to the atmosphere. In addition, if CCS is coupled to bioenergy process, capturing the so-called biogenic carbon (produced from biomass processing and already absorbed through photosynthesis process), we have the so-called BECCS process (Bioenergy and Carbon Capture and Storage), which can allow bioenergy production and use processes to achieve a negative carbon footprint. Therefore, the objective of this study is to evaluate the importance of applying BECCS technologies in the Brazilian sugar-energy sector, together with the existing challenges of such process.

Methodology: The methodology used was a case study of a mill with a medium-sized sugar cane milling capacity. The potential for CO2 capture was estimated using the mass balance of the processes involved. The required information was assessed from scientific publications, including reports from ANP (National Agency for Oil, Gas and Biofuels) and EPE (Energy Research Company) reports.

Preliminary results: Considering mills with sugarcane milling up to 1.6 million tons per season, producing only ethanol, as well as the process waste for biogas production and its use for electricity generation, the maximum estimated technical potential for CO2 capture is 734,444 tons per harvest. From this total, 13% comes from the fermentation process, 80% from sugarcane bagasse burning and 7% from biogas burning for electricity generation. When biogas is upgraded to produce biomethane, the estimated technical potential for CO2 capture is 708,626 tons per season, from which 14.1% comes from the fermentation process, 82.9% from bagasse burning and 3% from biogas upgrading.

Preliminary conclusions: Despite presenting the highest potential for BECCS, post-combustion CO2 capture presents an energy penalty that can consume between 15 and 20% of the energy produced. Although the technologies used for this CO2 capture process, such as absorption in solvents or solids, have a high TRL (Technology Readiness Level) in the 8 or 9, further developments are required to reduce the energy penalty and, consequently, the cost of such post-combustion capture.

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Abstract Title: Hormonal signaling network can contribute to design strategies to improve sugarcane growth and yield

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Abstract: Sugarcane is an essential crop in the Brazilian agricultural scenario, mainly used as

a feedstock for sugar and bioethanol production, contributing to mitigate carbon emissions. Attention to the production of biofuels has led to a scientific advance in understanding sugarcane physiology, biochemistry, and molecular biology. Integrating the sugar sensing and signalling processes with hormonal networks systemically helps design strategies to modulate plant growth, increase yield, and adapt to different climatic conditions. Here, we employed biochemical analyses to determine the levels of polyamines (PAs), amino acids, abscisic acid (ABA), and indole-3-acetic acid (IAA) in leaves and culms of sugarcane. Also, a bioinformatic analysis was performed to identify a set of genes related to these biosynthesis and hormonal signalling pathways. PAs were most abundant in leaves, particularly putrescine. The most abundant amino acids were ornithine and lysine in leaves and asparagine, glutamine, and histidine in culms. High levels of hormones IAA and ABA were detected in leaves during the last month of sugarcane development. A deep search by genes related to receptors and signalling of ABA, BR signalling, PAs-, ethylene- and amino acids-biosynthesis allowed the recovery of 3042 sequences from 7 sugarcane databases (transcriptomes and genomes). After restrictive filtering (coverage, presence of domains, and removing redundant sequences), 784 candidate sequences remained corresponding to 36 groups of genes from the pathways described above. In silico expression profiles revealed that genes related to PAs biosynthesis and ABA- and BR-signalling were the most expressed in two sugarcane transcriptome datasets (root development and stress conditions). These findings could be used to genetically modify sugarcane to accelerate growth and sugar accumulation.

Keywords: hormones signalling, growth, carbon, bioenergy, metabolism.

Introduction and Objectives: Integrating the sugar sensing and signalling processes with hormonal networks constitutes a strategy to increase the capacity and resilience of crops to extreme environmental conditions. In this way, is fundamental to understand the plant hormones signalling pathways through studies that promote a better knowledge of stress responses, cell wall structure, and energetic metabolism. The integrative plant perception and management of carbohydrates and other metabolites could serve as a control mechanism to integrate external environmental factors, nutrient homeostasis, developmental programs, and stress response to anabolic and catabolic processes. In this core, amino acids and plant hormones pathways [including polyamines (PAs), brassinosteroids (BRs), abscisic acid (ABA), auxins as Indole-3-acetic acid (IAA)], as well receptors and signalling components act in concert in numerous plant physiological processes, which determine the cell fate and differentiation, tissue and organ development, or environment responses. This complex network can lead to the breeding of important crops used as sources of food or bioenergy, such as sugarcane. Sugarcane is an important crop in Brazilian agriculture and bioenergy scenarios and a broader physiological and molecular coverage can aid in understanding its metabolism, helping to elucidate the metabolic pathways that influence crop gain of yield. Here, the identification and characterization of the biochemical and molecular variation in the hormonal signalling components in sugarcane is reported. This study includes plant hormone and amino acid profiles in a sugarcane growing in the field during 12 months, and the identification of a

set of genes expressed in sugarcane under different conditions. For this, two strategies were employed: i) a biochemical profile during sugarcane development in the field, and ii) identification and characterization of genes related to receptors and signalling of ABA, BR signalling, PAs-, ethylene- and amino acids biosynthesis, in two sugarcane transcriptome datasets.

Methodology:

Plant material:

Green fully expanded leaves and culm from sugarcane plants grown in the field were collected in 01, 03, 06, and 12 months of development, according to De Souza et al. (2018). The plant material was ground in liquid nitrogen and used for biochemical characterization.

Biochemical analysis:

Putrescine, spermidine, and spermine were extracted according to de Oliveira et al. (2018). Samples were homogenized with cold 5% of perchloric acid and subjected to three cycles of freezing and thawing. After centrifugation, the supernatants containing the free PAs were collected and derivatized. Dansylated PAs were extracted with 200 µl of toluene and the supernatant was collected and dried under nitrogen. Dansylated PAs were dissolved in 200 µl of acetonitrile.

The extraction and determination of free amino acids were performed according to de Oliveira et al. (2018). Aliquots of fresh material were extracted with 80% ethanol. Amino acid derivatization was realized with o-phthalaldehyde.

The hormones ABA and IAA were extracted and quantified according to Álvarez-Florez et al. (2017) and Silveira et al. (2008), with modifications. Fifty mg of the dry weight of leaves and culms were homogenized in 2.5 ml extraction buffer containing methanol and isopropanol (20:80), 1% acetic acid, and 0.5 µCi.ml-1 of [3H] IAA and [3H] ABA (internal standards).

The metabolites were separated by HPLC on a reversed-phase C18 column (5 µm x 4.6 mm x 250 mm). PAs were detected at 340 nm (excitation) and 510 nm (emission) wavelengths with a RF-20A fluorescence detector. ABA content was determined using a UV-VIS detector at 254 nm, while IAA content was determined using a fluorescence detector at 280 nm (excitation) and 350 nm (emission).

Bioinformatic analysis:

A bioinformatic approach was employed to identify a gene set related to PAs-, ethylene- and amino acids-biosynthesis, and ABA and BR signalling pathways. The main genes comprising these networks (receptors, transcription factors, and enzymes) were first identified and characterized in model species (Arabidopsis, rice, and maize), through Tair, Phytozome, Rice Genome Annotation, and Maize Genomics Resource platforms. These sequences were used as queries to identify and recover sequences from seven sugarcane databases (transcriptomes and genomes). Restrictive filtering including coverage and presence of domains, as well as the removal of redundant sequences, were employed to maintain those reliable sequences with high

identity. Sequences were grouped through EGGNOG code related to domains annotated in the EGGNOG platform.

In silico expression analysis (CPM values) were performed by using two sugarcane transcriptome datasets: i) from four segments of roots, during aerenchyma development; and ii) from sugarcane plants growing under stress conditions (control, drought, elevated CO2, or by a combination of them). A heatmap and Hierarchical cluster by Euclidean distance was performed using the CPM expression values.

Preliminary results:

PAs, amino acids, and hormonal profiles in sugarcane field:

In all months analysed, PAs were most abundant in leaves. The content of each PA in the leaf and culm revealed that the highest amount in the total PAs during month 01 was caused by putrescine and spermidine, respectively. Putrescine was the main PA in the leaf along the sugarcane development, followed by spermidine and spermine. During the sugarcane development, the amino acid content was more constant in the leaf than in the culm, in which the total amino acid levels were 12 times higher in the month 01. The most abundant amino acids found in the leaves were ornithine and lysine, whereas in culm were asparagine, glutamine, and histidine. Sugarcane leaf and culm have different IAA and ABA profiles during development, especially concerning IAA abundance, which was much higher in the leaf at most time points analysed. High levels of hormones IAA and ABA were detected in leaves during the last month of sugarcane development. In silico mining of hormonal signalling network in sugarcane

A deep search by genes related to receptors and signalling of ABA, BR signalling, PAs-, ethylene- and amino acids-biosynthesis, allowed recovery of 3042 sequences from 7 sugarcane databases. This amount is 18, 23, and 25 times more than found in Zea mays (170 sequences), Oryza sativa (132 sequences), and A. thaliana (120 sequences), respectively. After restrictive filtering, 784 candidate sequences remained corresponding to 36 groups of genes from the pathways described above. A search on two sugarcane transcriptome datasets realized by Lafieco's group was performed to recover both sequence and expression values (CPM). In the root transcriptome dataset, 454 sequences were expressed in the four root segments, and 240 were differentially expressed (DEG) among the segments. In leaves from sugarcane growing under different stress conditions, 260 sequences were expressed, and 65 were DEGs. PA biosynthesis/catabolism pathways and members related to the SnRK2 subfamily were the pathways with the greatest number of genes.

In silico expression profiles revealed the pattern of the primary genes expressed in this hormonal signalling network. In root transcriptome, genes related to PAs biosynthesis and catabolism (SAMS, SAMDC, SPDS/SPMS, ALDH, and CuAO), SnRK2, and ABA- e BR-signalling genes were the most expressed genes in all root segments. Ethylene biosynthesis genes (ACS and ACO) are low expressed, suggesting that methionine is directed to PA biosynthesis during the root development. In the sugarcane stress experiment, genes related to spermidine and spermine biosynthesis (SAMS, SAMDC, SPDS/SPMS) are slightly more expressed under elevated CO2 conditions. Most genes involved in ethylene biosynthesis genes

are low expressed under these conditions. Genes related to ABA signaling (PP2C-A) and proline biosynthesis (P5CS1/2) showed high expression values, indicating their participation in the stress response.

Preliminary conclusions: In summary, this study allowed a detailed analysis of hormonal signalling network components in sugarcane plants by two strategies: i) a biochemical profile during sugarcane development in the field, and ii) through identification and characterization of genes related to receptors and signaling of ABA, BR signaling, PAs-, ethylene- and amino acids-biosynthesis, in two sugarcane transcriptome datasets. In the first strategy, biochemical analyses revealed different profiles between the two organs analysed (leaves and culm), and also during the sugarcane development in the field. These changes provide insights into distinct metabolic profiles of each organ throughout development and pave the way for a more integrative understanding of the biological functioning of sugarcane in the field, which can contribute to future strategies to improve yield performance. In the second strategy, the main set of genes involved in hormonal signalling in sugarcane was identified. Differentially expressed genes were observed in each transcriptome dataset analysed, demonstrating variations among PAs biosynthesis and catabolism, and ABA- and BR-signalling. These differentiated responses to stresses will be assessed by physiological measurements (hormonal, amino acids, carbohydrates, and biomass profiles) in sugarcane overexpressing the gene RAV (RELATED TO ABI3/VP1), which is induced by a balance between auxin and ethylene, and lead to a repression effect on the EPG1 (ENDOPOLIGACTURONASE1), involved in the expression of pectinases genes. This study allows a detailed analysis of the partial core hormonal signalling components in sugarcane and these findings provided suitable targets for genetic engineering in sugarcane to accelerate growth and sugar accumulation.

André Henrique Baraldi Dourado
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Abstract Title: Lignin Oxidation on CuO: (Electro)chemical Approaches

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Abstract: Lignin is a macromolecule that is found in biomass, but it has limited industrial applications. It is a byproduct of the pulp and paper industry or bioethanol production and is mainly used as fuel for thermoelectricity production. However, lignin is the most abundant renewable aromatic compound which turns it in a promising source of high added value aromatic chemicals. Therefore, there is a high interest in investigating the catalytic depolymerization of lignin to obtain these products. CuO is a potential candidate for heterogeneous catalysis to obtain monoaromatic phenol molecules with ketonic or aldehydic

carbonyl, or carboxylic acids in para position, at high temperatures of up to 180 ºC and high O2 pressures. The resulting products may have zero, one, or two methoxy groups, -ortho to the phenolic hydroxyl, depending on the starting macromolecule's monomeric distribution. Cu oxides are known in electrochemical literature to be good oxidative catalysts in alkaline media. This approach can not only find a new way to oxidize lignin, but also provide insights of this catalyst for lignin oxidation. The electrochemical approach produces the same monoaromatic products observed in heterogeneous catalysis, including a similar proportion of functional groups in para. After quantifying the monoaromatic products from the oxidation using gas chromatography, we calculated that the Faradaic efficiency at 1.65 VRHE is 28%. The catalyst was electrochemically characterized by electrochemical impedance spectroscopy and capacitive cyclic voltammetry for investigating changes in surface area and oxide characteristics using multi-frequency Mott-Schottky analysis (mf M-S). This analysis showed a decrease in the charge carrier density of this n-type intrinsic semiconductor, which was dependent on the oxidation potential applied. This suggests that these species are involved in the electrochemical mechanism and probably in the heterogeneous one as well. Raman spectroscopy and scanning electronic microscopy were used to compare changes in chemical/crystallographic structure and morphology when the catalyst was applied in heterogeneous and electrocatalysis.

Keywords: Electrocatalysis, Thermocatalysis, Electrobiorefinery, Biorefinery, Mott-Schottky

Introduction and Objectives: To obtain data that can relate the thermo- and electrocatalytic lignin oxidation, and investigate the reaction mechanism of these two paths by electrochemical in situ analysis

Methodology: Electrochemical techniques such as triangular and step potential perturbation, electrochemical impedance spectroscopy, product analysis by gas chromatography and material characterization by scanning electronic microscopy, and Raman spectroscopy by ex situ, for the thermal material and in situ for the electrochemical.

Preliminary results: Electrochemical and thermochemical heterogeneous catalyse produced the same products at similar yields, considering the faradaic and mass ones, in order. That suggested that the same mechanism was observed, specially due to the fact that for both approaches there is an optimum oxidative power for this selectivity. The optimum conditions were followed, in both cases, by a diminishing in particle size and narrowing in the Ag Raman signal. The first observation was related, by electrochemical impedanc spectroscopy, to an enhancing in oxygen vacancy population, which was understood as the reason for the later phenomenon. The oxygen vacancy population increment was understood to be the reason for the catalytic activity and selectivity to aldehydes.

Preliminary conclusions: Electrochemical techniques can provide novel information about thermocatalytic processes, especially when spectroscopic techniques are used as a bridge

between both approaches. Oxygen vacancies were understood as the active sites for the catalysis.

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Abstract Title: Computational Engineering Approaches for Geologic Carbon Storage Site Qualification in the Brazilian Context

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Abstract: Site qualification represents an intermediate phase within the geologic carbon storage workflow, dedicated to the identification of subterranean areas characterized by favourable petrophysical properties, along with desirable storage capacity, injectivity, and containment attributes. Over recent decades, numerous nations have successfully instituted facilities and technological frameworks for carbon dioxide (CO2) storage, guided by well-defined site selection and characterization protocols. Nonetheless, the application of these protocols within the Brazilian context is in its nascent stage and necessitates further development. This study leverages computational engineering tools to formulate a suite of data- and simulation-driven models with the primary objective of furnishing quantitative assessments for the evaluation of potential CO2 storage sites, with particular relevance to forthcoming Geologic Carbon Storage (GCS) initiatives in Brazil. The principal focal points of our investigation encompass the following challenges: the construction of mathematical functionals to elucidate the overall quality of porous media, the deployment of machine learning algorithms for rock type classification, and the execution of well placement and long-term numerical simulations of CO2 injection to gain insights into gaseous fluid dynamics. Preliminary findings applied to a well-established Brazilian reservoir model demonstrate that the proposed methodologies yield advantageous storage attributes in comparison to select benchmarks, thus holding promise for the qualification of CO2 storage sites.

Keywords: Geologic carbon storage, site selection, reservoir characterization, modelling and simulation, computational methods.

Introduction and Objectives: Currently, geologic carbon storage (GCS) stands as a pivotal confluence of technologies, critical for the mitigation of carbon dioxide (CO2) emissions and

the facilitation of the global transition towards a carbon-neutral paradigm. Serving as a foundational precursor to the implementation of GCS, site qualification emerges as a critical step to ensure that appropriate locations, such as depleted oil and gas reservoirs, inactive coal deposits, and aquifers characterized by substantial storage capacity and enduring security, are judiciously selected for project deployment. As of the close of 2022, the annual rate of CO2 storage reached around 40 million tonnes. Across the globe, numerous GCS ventures have achieved noteworthy success, with notably growing commercial viability, particularly in regions such as Australia, North America, the North Sea area, and the United Kingdom. Nevertheless, GCS initiatives within the Brazilian context remain in their infancy, marked by few numerical investigations at the geological formation level. Despite harboring an offshore storage capacity of approximately 3121 MtCO2, GCS projects in Brazil remain an emergent frontier, poised for substantial growth after the recent regulatory milestones. While numerous studies have introduced site screening, selection, and characterization workflows for the evaluation of GCS potential, their applicability within the Brazilian landscape remains at an incipient stage. In the present study, we provide a comprehensive suite of simulation-based qualification functionals and data-driven methodologies destined to qualify storage sites in terms of containment efficiency. These functionals are mathematical models that combine diverse physical parameters employed for strategic well placement and useful for long-term injection simulations. Our findings show that storage sites with potential containment are detectable through these novel functionals.

Methodology: The methodological framework encompasses a comprehensive set of techniques, including grid modelling, structural trap analysis, mathematical modelling, and numerical simulations. Our numerical experimentation is conducted utilizing the well-established UNISIM-I-D model for the sandstone reservoir Namorado, situated in the Campos Basin. We develop mathematical functionals, achieved through the amalgamation of pertinent petrophysical properties. These properties encompass the reservoir process speed, flow deliverability function, and trap-to-catchment volume ratio, all of which are essential for the assessment of site viability. Furthermore, our approach incorporates the concept of discrete dynamic units, along with injectivity unit classes and clustering methods that improve well placement. Under the volumetric quality map methodology, we employ binning techniques, partitioning, and Jaccard index cutoffs to discern optimal site locations. For the execution of CO2 injection simulations, we employ the MRST-co2lab module, tailored for use with Matlab. These simulations are grounded in a comprehensive two-phase gas-brine model coupled with a Darcy flow model, which facilitate a comprehensive exploration of the CO2 dynamics and plume diffusion.

Preliminary results: The initial findings from our study have revealed that wells strategically positioned in accordance with the functionals proposed have yielded notably superior results in terms of CO2 capture during simulation scenarios spanning 100 years of injection and 1900 years of gas migration, as opposed to legacy wells and parametric groups existing in the

literature. In a few instances, the surplus storage capacity achieved increased up to 50%.

Preliminary conclusions: This study marks a pioneering application of computational engineering resources within the context of site qualification in Brazil. We have provided a robust mathematical framework to elucidate containment efficiency at the geological formation level. Our analyses indicate that the storage efficiency improves when compared to established benchmarks. From a numerical perspective, our research holds considerable promise as a decision support tool for guiding new geologic carbon storage projects in Brazil.

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Abstract Title: Carbon Capture Utilization and Sequestration in Basaltic Rocks from The Serra Geral Formation: A Petrographic Characterization Before and After the Co2 Injection

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Abstract: The carbon capture utilization and sequestration is an important tool to deal with the problems caused by the global warming, motivating scientists around the world to research ways to reduce/mitigate its effects, especially in the Carbfix (Iceland) and Columbia River (United States) initiatives, the main projects that study the CCUS tool. Here in Brazil, a joint initiative bewteen the REPSOL company and a few universities started to develop its own CCUS methodology. Here in the São Paulo state, in the outskirts of city of Ribeirão Preto, tholeiitic basaltic samples of the Serra Geral Formation in the Parana Basin were collected in four quarries by the USP team. The mineralogy of these basalts are mainly composed by Ca-plagioclase (labradorite), Ca-pyroxene (augite), zeolite (laumontite), with quartz and opaques (oxides) occurring as secondary minerals. After the field work, the samples were attacked with a combination of CO2 and NaOH and after the x-ray diffraction analysis, if carbonates were formed, the rocks were analyzed to understand how the carbonation worked. This happened in the sample collected in the CGS quarry, in which were generated as products of this injection mainly dolomites enriched in iron, due to the Fe content present in the sample originally. Albite (as an anorthite pseudomorph) and quartz were also formed as results from the CO2 + NaOH injection in the reaction with the samples. Now the injection for the next analyses with samples collected by the PUC from the Rio Grande do Sul state will be only attacked with CO2 in aqueous form, with the objective of testing and evaluating the effectiveness of the CO2 injections in the IND quarry and the other basalt samples from the PUC-RS university.

Keywords: CCUS, Serra Geral Formation, tholeiitic basalts, Fe-enriched dolomites.

Introduction and Objectives: Carbon capture utilization and sequestration (CCUS) is being an important tool for the mitigation of the global warming malicious effects in all the world. Here in Brazil, inspired by the Carbfix and the Columbia River CCUS projects (both in Iceland and in United States, respectively), a team composed by a few universities (USP, UnB and the PUC-RS; from the Rio Grande do Sul state) alongside with the REPSOL company was formed with the objective of determine the CO2 storage inside basaltic rocks of Brazil, especially in the Serra Geral Formation of the Paraná Basin, in which is present in states of south, southeastern and center-west regions in Brazil, one of the largest igneous provinces in the world. These dimensions represent a great potential of CCUS use. In the USP, in which this

work was (and is) based, it was conducted a field work in which collected tholeiitic basaltic samples from four quarries (Inderp, CGS, Carrascoza and Borborema) near the city of Ribeirão Preto, within the São Paulo state, with the objective of develop a petrographic characterization of this samples before and after the CO2 injection in the basalts, understanding these carbonation processes and its effectiveness.

Methodology: For the CO2 injections in basalts, it was used the following protocol: 1) The sample was injected with a combination of CO2 + NaOH. 2) After that, through x-ray diffraction analysis we determine if the carbonation happened. 3) If the carbonation happened, other analysis such as MEV, EDS, ICP-MS, TGA, XRF and BET were performed for the development of the petrographic characterization. For the next analyses, however, the substance injected will be composed only with CO2 in aqueous form.

Preliminary results: Initially, according to the XRD analyses performed, there was no carbonation, with exception of the IND (Inderp) quarry, in which were observed some phases with a good correlation with cancrinite, a hydrated carbonate formed probably through the CO2 attack in Na-plagioclase present in the basalts. The percentage of the cancrinite wasn't very expressive, however, and will be analyzed by MEV and other analytical methods mentioned in the Methodology topic. The sample of the CGS after the mineralization presented a predominance of dolomite phases according to the XRD analysis. With the carbonation observed the protocol for the samples analyses was followed, and with the MEV, EDS and TGA analyses it was possible to notice the presence of dolomite enriched in calcium, magnesium and iron because of the presence of oxides, labradorite, laumontite and augite in the sample before the mineralization.

Preliminary conclusions: The injection of CO2 + NaOH was successful, but only for two of four samples (and in the Inderp case there aren't many phases with good correlation with the XRD pattern of the sample) the carbonation happened. Now with the injection of CO2 it can be observed with the next samples analyses provided from the PUC-RS university how effective the carbonation reactions will be.

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Abstract Title: Solvent-Free Hydrogenation of Succinic Acid into Tetrahydrofuran

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Abstract: Succinic acid (SUC) is an important building-block molecule in the production of various high-value added products, like tetrahydrofuran (THF). For this reason, the present study aimed to investigate the hydrogenation of succinic acid in a solvent-free media using using bimetallic nanostructured catalysts of palladium and rhenium supported on silica (PdRe/SiO2). The impact of hydrogen pressure, temperature and mass of catalysts on the catalytic performance was evaluated using an experimental design. The evaluated parameters had little impact on SUC conversion, which remained approximately 100% under all tested conditions. In contrast, the temperature and catalyst mass had a significant influence on the reaction's selectivity, achieving a 73% selectivity for THF. This result is very promising, considering that it is a solvent-free reaction medium based on in environmentally friendly processes.

Keywords: Hydrogenation, succinic acid, tetrahydrofuran, environmentally friendly processes.

Introduction and Objectives: Succinic acid (SUC) is an important building-block molecule in the production of various high-value added products, like tetrahydrofuran (THF). For this reason, the present study aimed to investigate the hydrogenation of succinic acid in a solvent-free media using using bimetallic nanostructured catalysts of palladium and rhenium supported on silica (PdRe/SiO2). The impact of hydrogen pressure, temperature and mass of catalysts on the catalytic performance was evaluated using an experimental design.

Methodology: The impact of hydrogen pressure, temperature and mass of catalysts on the catalytic performance was evaluated using an experimental design.

Preliminary results: The evaluated parameters had little impact on SUC conversion, which remained approximately 100% under all tested conditions. In contrast, the temperature and catalyst mass had a significant influence on the reaction's selectivity, achieving a 73% selectivity for THF.

Preliminary conclusions: This result is very promising, considering that it is a solvent-free reaction medium based on in environmentally friendly processes.

0911 – GHG23 (TV3)

Chairs: Renato Picelli – Marcelo Sekler

Fernanda de Marco de Souza
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Abstract Title: GHG emissions in wastewater treatment plants: nitrous oxide and the importance of data collection and monitoring

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Abstract: Greenhouse Gas (GHG) emissions from Wastewater Treatments Plants (WWTPs) is a recent topic that requires attention. The treatment of domestic effluents can emit GHGs directly and indirectly. When it comes to nitrous oxide, WWTPs emit mainly from biological nitrogen removal processes, and their emission can be reduced by adopting ideal operational parameters. Thus, it is important to check the monitoring data that the stations already have available and to draw associations. Also, a systematic review of the literature is being conducted on the topic. The months and operating ranges that have the greatest potential for emissions were verified. The relationships were observed based on data already measured by the WWTPs. Furthermore, there has been an increase in publications on the topic in recent years, showing that such observations and knowledge need to be communicated to decision makers. Therefore, it is important that dialogues between sanitation companies and universities are intensified, as well as the relevance of systematizing and processing the WWTP's operating data. Finally, a summary guide with causes and mitigation strategies is being finalized.

Keywords: GHG, WWTPs, nitrous oxide, mitigation.

Introduction and Objectives: The increasing concentration of Greenhouse Gases (GHG) in the atmosphere is a global and emerging concern. Within this context, it is highlighted that the treatment and disposal of domestic and industrial wastewater are among the sources of GHG emissions [1,2]. In the treatment of domestic effluents, Wastewater Treatment Plants (WWTPs) can emit directly and/or indirectly, including energy consumption and the water treatment process itself [3], of which methane and nitrous oxide stand out. Reducing the use of non-renewable resources, minimizing waste generation and using the resources that are generated in the treatment process are actions that WWTPs can implement to improve their sustainability [4]. Another aspect is being able to directly contribute to the mitigation of climate change. WWTPs are sources of N2O emissions, especially in the biological nitrogen removal stage

(nitrification denitrification), which presents a greater or lesser degree of emission depending on the parameters and operational conditions adopted. Emissions vary depending on internal factors, such as: temperature, dissolved oxygen concentration and changes in pH [5,6]. Optimized operational parameters: dissolved oxygen, pH and temperature can be established to reduce emissions. Furthermore, monitoring nitrogen compounds throughout the process, as well as available organic matter, are also important for managing and estimating possible emissions. Based on this, we sought to examine operational data from WWTPs in the Metropolitan Region of São Paulo on a full scale with the purpose of establishing associations between operational variables and points of attention in operational control.

Methodology: Using data from the WWTPs, it was possible to characterize the raw and treated sewage and related to the treatment stages, as well as verify associations between the variables. The data were processed using descriptive and inferential statistics – correlation coefficient. Spearman's rho coefficient (ρ) was adopted and the interpretation of correlation coefficients. All analyses were carried out using IBM SPSS Statistics software.

Preliminary results: The months throughout the year and operating ranges with the greatest potential for the formation and emission of nitrous oxide. In one of the WWTPs, for example, during the months of August-October there were high concentrations of ammonia flowing into the tanks. Ammonia is directly related to the production of N2O, so there are greater chances of its formation the higher the concentrations of Ammonium-N available for conversion into nitrite and nitrate. The decrease in dissolved oxygen levels combined with higher nitrate concentrations can favour the formation of nitrous oxide both from the inhibition of nitrification and as an intermediate product of heterotrophic denitrification. It was possible to estimate the influent nitrogen load and from this determine how much could be avoided from being emitted into the atmosphere. These relationships were created based on data already measured and made available by WWTPs. Within this context, the importance of monitoring and optimizing operations throughout the wastewater treatment process is highlighted.

Preliminary conclusions: Therefore, for WWTPs to move towards greater sustainability (reduction of emissions, but also reinsertion and use of generated resources) it is necessary to have a systematic collection and treatment of operating data - including concentrations and quantities throughout the treatment process -, contributing to the management and reduction of the carbon footprint.

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Felipe Silva Maffei
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Abstract Title: Design of smart labyrinth seals for mitigation of GHG emissions in pneumatic machines

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Abstract: In this work a topology optimization model for designing optimized labyrinth seals is proposed. The model consists of compressible and turbulent flows in an axisymmetric domain coupled with a boundary propagation model. Propagation is used to impose different solid behaviours based on which wall it is connected to, i.e., solid material in contact with the shaft will have a rotational velocity, while material encrusted in the support will have zero absolute velocity. The implementation is composed of a segregated solver with steps for the FANS equations, the k-epsilon turbulent equations, and the propagation model. The sensitivity is obtained with automatic differentiation of the adjoint method. The IPOPT optimizer is used to solve three different objective functions, maximization of radial velocity, static pressure, and Q-criteria. The results are designs for small scale labyrinth seals in real operation conditions.

Keywords: Compressible, Turbulent, Topology Optimization, Labyrinth Seal, Finite Element.

Introduction and Objectives: Human activity on the global climate system has been the vector of extreme events and accelerated changes in the mean global temperature. One of the highly alarming consequences is triggering climate tipping points, that is, perturbations on climate systems that become self-exciting. In this scenario, the changes may occur faster than beyond human adaptivity, and the new equilibrium point becomes irreversible. In the face of such an alarming scenario, the United Nations (UN) elaborates a plan of action containing 17 points to shift the world toward a sustainable future. In particular, subtopic number 9.4 is concerned about the increase of industry efficiency, and adoption of clean technologies in which the scope of the present paper can be included, i.e. the optimization of labyrinth seals. Labyrinth seals are replaceable structures positioned between zones of high pressure and low pressure aiming to reduce the flow that rises due to this pressure difference and the clearance between the rotating parts and static parts in turbomachinery devices. The main occasions where is necessary the application of LS is in the separation of stages of compressors (or turbines), and in separating the atmosphere from the inner region of the compressor (or turbines). The working principle is straightforward. Its geometry is designed in such a way to create the most tortuous, but still manufacturable, path along its length, with no parts from the rotating shaft touching the static shell. The consequence is a flow path with significant pressure head drop, but still with a small leakage. Its characteristics make this leakage an inherent consequence of this type of seal, thus, even the most efficient labyrinth seal will have it. In spite of the inherent leakage, the labyrinth seals are a preferred industrial solution because of their reliability, there is no contact between the rotating and static parts (avoiding problems with erosion), ease of maintenance, and it is a cheap solution. However, depending on the type of gas the compressor operates, the leakage (from the inner of the compressors to the atmosphere) makes the machine a greenhouse gas (GHG) source. Among the possibilities, the emissions related to methane (CH4) are of particular interest once they become a preference target to combat climate change since COP26. This is because CH4 is significantly more potent to cause warming (around 80 times \cite{methane2023}) and has a reduced half-life (12 years) when compared to carbon dioxide (20 years). Most of the literature works use parametric optimization to enhance the design of LS and just recently the first works applied topology optimization methodology. However, this work treats the incompressible laminar or incompressible turbulent flow regime. The present work proposes to apply topology optimization to the labyrinth seal problem considering the turbulence and compressibility of the flow.

Methodology: This work considers a steady-state, compressible, turbulent 2D-swirl model with axisymmetric. In order to consider the eddy viscosity turbulent approximation in the Navier-Stokes (NS) equations, usually, the Reynolds Averaged NS (RANS) are used. However, in compressible flows, an additional approximation is used for the density fluctuation. This is done with the Favre-Averaged NS equations (FANS), which account for the effects of turbulence by averaging over the turbulent fluctuations with the density and provide a statistical description of compressible flow fields. The turbulence model selected to close the set of

equation is the k-epsilon model. This one describes an approximation for the turbulence kinetic energy (k) and the turbulence dissipation rate (ε), using empirical constants to adjust the model. The β-propagation model is used to propagate prescribed values of boundaries into solid region ($\alpha = 0$) that are in direct contact with. While, in fluid regions ($\alpha = 1$) the model forces a fixed value of $\beta = 0$. In this case the propagation technic is used to propagate the rotating wall from the axis through the solid connect with it. In order to consider the axisymmetric, a cylindrical coordinates frame is considered. The FANS equations are used in the absolute stationary frame and the rotation is imposed by the boundary conditions. The topology optimization method involves distributing material over a specified domain by following certain requisites. In the fluid flow problem, introduced a porous domain dividing domain region between high permeability material, interpreted as pure fluid, and low permeability material, representing solid by using an absorption term κ. The interpolation used is proposed by Borrvall and Petersson. The objective function proposed to this work is the maximization of radial velocity.

Preliminary results: The first results are related to the maximization of the radial velocity. The objective function showed to be able to increase the viscous loss and at the same time ensure gap between the rotation and static parts of labyrinth seal.

Preliminary conclusions: The topology optimization was successfully applied in the design of labyrinth seal. The maximization of radial velocity was able to produce a geometry which dissipates the energy while ensuring a gap between the rotating and static parts of the seal. The resultant geometry has a shape, indicating that the usual manufacturing methods will not be able to manufacture the seal. To tackle this problem, the addictive manufacturing could be used.

Emilio Carlos Nelli Silva
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Abstract Title: Design of smart labyrinth seals for mitigation of GHG emissions in pneumatic machines (compressors and turbines)

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Abstract: The emission of Greenhouse Gases (GHG), mainly CH4 and CO2, is a main contributor to global warming. This makes it a core part of the climate change conferences (such as COP27) and agreements (Kyoto Protocol and Paris Agreement). Furthermore, it is an integral part of the Sustainable Development Goals (SDGS). One important contribution to the emission of GHG are turbomachines (compressors and turbines), which contain seals between the case and the shaft, in order to separate the high pressure inside the turbomachine to the low pressure outside the turbomachine, in order to reduce the imminent leakage through this gap. The most commonly used seal is the Labyrinth Seal (LS), which is contactless between the case and the shaft. This project aims to integrate smart materials in LS design creating the concept of smart LS aiming to achieveminimum GHG emissions in pneumatic machines. Current LS designs include mostly (or only) passive parts and intuitive geometries; therefore, this project aims to create the concept of smart LS with active materials and innovative geometrical features. Some preliminary results are presented, the formulation is still being improved, concepts are being tested, the test bench is being calibrated, and some tribology studies have been performed.

Keywords: Labyrinth seal; Smart materials; Topology optimization; CFD; Experimental validation; Tribology.

Introduction and Objectives: This project aims to integrate smart materials in Labyrinth Seals (LS) design creating the concept of smart LS aiming to achieve minimum Greenhouse Gases (CH4 and CO2) emissions in pneumatic machines. Current LS designs include mostly (or only) passive parts and intuitive geometries; therefore, this project aims to create the concept of smart LS with active materials and innovative geometrical features. The objectives of this project are: to integrate smart materials in the LS design, to consider the influence of parameters in the smart LS concept such as high shaft speed (order of 20,000 rpm and shaft radius 40 to 60 mm), different types of SMA actuation and possible configurations of smart LS; to consider turbulent flow in the topology optimization LS design; to create a schematic methodology for smart LS design; to manufacture and test prototypes comparing smart LS designs with traditional LS designs; to perform wear studies of smart LS designs.

Methodology: The project is being tackled through many fronts, and include: the design of LS through the topology optimization method, involving turbulent flows, turbulent compressible flows, fluid-structure interactions and dynamic fluid interactions, in order to achieve innovative formats; computational fluid dynamics; the use of smart material for LS; experimental bench and tests; and tribology studies. Thus, the main challenging points are: the topology optimization considering turbulent flow, compressible turbulent flow, and new innovative LS configurations; the test bench, which is initially being tested, adjusted and calibrated before conducting the aimed experiments; the use of Nitinol for the smart LS concept; and tribology and wear studies.

Preliminary results: The topology optimization for LS was explored with various adaptations and concepts in the formulation, although these and other new concepts and the turbulent and compressible turbulent effects are still under research. The validation of these innovative designs is to be performed experimentally through a test bench, which has been fabricated, and is now being Preliminarily tested, adjusted and calibrated. preliminary tests and simulations were performed with Nitinol for the smart LS concept, and are is still ongoing. Tribology and wear studies were also performed for LS, showing how wear happens in some traditional LS designs.

Preliminary conclusions: The topology optimization for turbulent flow, as well as for turbulent compressible flow and related physics and interactions are still being investigated, as well as other new concepts and optimization strategies. The test bench is initially being tested, adjusted and calibrated before conducting the aimed experiments. The use of Nitinol is currently being investigated for the smart LS concept and seems promising. Tribology and wear studies are also being performed, showing how wear happens in LS.

Renato Picelli
University of São Paulo (PNV)

Abstract Title: Efficient Turbulent Fluid-Structure Topology Optimization with Smooth Boundaries Using Sequential Integer Linear Programming

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Abstract: Topology optimization methods face serious challenges when applied to structural design with fluid structure interaction (FSI) loads, especially for high Reynolds fluid flow, i.e., considering turbulence. In this problem, the information at the fluid-structure interface is crucial for the modelling and convergence of the turbulent fluid flow analysis. This work devises a new explicit boundary method that generates two- and three-dimensional smooth surfaces to be used in topology optimization with binary {0,1} design variables. A phase-field function is obtained after nodal spatial filtering of the design variables. The 0.5 isoline defines a smooth surface to

construct the topology. The FSI problem can then be modelled with accurate physics and explicitly defined regions. The Finite Element Method is used to solve the fluid and structural domains. This is the first work to consider a turbulent flow in the fluid structure topology optimization framework. The fluid flow is solved considering the k-ϵ turbulence model including standard wall functions at the fluid and fluid-structure boundaries. The structure is considered to be linearly elastic. Semi-automatic differentiation is employed to compute sensitivities and the optimization problem is solved via sequential integer linear programming. Results show that the proposed methodology is able to provide structural designs with smooth boundaries considering loads from low and high Reynolds flow.

Keywords: Topology optimization; Fluid-Structure Interaction; Integer Linear Programming; Turbulence; High Reynolds flow.

Introduction and Objectives: Computational methods play an important role in engineering projects, particularly in the design of elastic structures. Often, simplifying the loads acting on a structure can led to efficient and practical designs. This simplification is achieved through techniques like analytical approximations, especially when dealing with loads from various physical sources. However, there are instances where loads are complex, design-dependent, and cannot be simplified or ignored due to the underlying physics governing the structure. Fluid-structure interaction (FSI) serves as a prime example of such scenarios. The infamous Tacoma Narrows bridge incident stands as a stark reminder of the consequences when fluid flows induce erratic motion and, ultimately, catastrophic failure due to dynamic loads. In this case, the structural layout was altered to accommodate changes in fluid flow, which led to unforeseen structural challenges. In today's engineering landscape, systems are growing increasingly intricate, and stringent economic and environmental demands necessitate structural designs and topologies that transcend intuitive approaches. This is particularly true in the context of FSI and the applications we are interested in the RCGI, such as pneumatic machines parts. Consequently, there is a pressing need for the development of new computational methods that can effectively address these evolving challenges in modern engineering systems. Addressing turbulent flow in topology optimization for fluid-structure interaction (FSI) is an exciting challenge. Existing methods have limitations, typically capping at Re = 120. To confront turbulence, we must explicitly define fluid boundaries and ensure smooth fluid-structure interfaces. This explicit definition is vital for solving turbulence equations efficiently. Conventional binary approaches often yield jagged boundaries that hinder turbulence simulations. In response, this research introduces an innovative 2D and 3D boundary smoothing technique. It cleverly combines binary design variables with explicitly smoothed boundaries. The primary goal is to optimize FSI systems while accommodating both laminar and turbulent flows, significantly expanding the practical utility of topology optimization in real world engineering scenarios.

Methodology: The solution of the fluid-structure governing equations follows a segregated approach, with separate domains, leveraging the capabilities of the commercial Finite Element

Analysis (FEA) software, COMSOL Multiphysics. Specifically, the Reynolds-Averaged Navier-Stokes (RANS) equations, along with the k-ϵ turbulence model, are resolved using standard wall functions within the software framework. For establishing equilibrium conditions at fluid-structure boundaries, such as wall functions, the Fluid Structure Interaction module within COMSOL Multiphysics is employed. To meet the demands of sensitivity analysis necessary for optimization, the semi-automatic differentiation module within COMSOL Multiphysics is harnessed. The proposed methodology revolves around a material distribution approach that hinges on a clear separation between the optimization grid and the FEA mesh. The integration of fluid-structure interaction and sensitivity analyses is achieved seamlessly through COMSOL Multiphysics. The optimization grid defines the design domain and begins with a binary topology, typically fully solid initially and transitioning to a solid-void configuration during the optimization process. Information about void regions or holes is extracted from the set of binary design variables. Initially, these contours exhibit jagged boundaries. Subsequently, these boundaries undergo a smoothing process facilitated by filtered binary design variables acting as phase field functions. In 2D, these are saved as .dxf files, while in 3D, they are saved as .stl files. Moreover, the smoothing contour procedure involves the application of a nodal filter to the distribution of design variables {0, 1}. This distribution transforms into a surface resembling a phase field function, representing filtered design variables composed of two phases: voids and solid. The solid phase ($\phi(xj) = 1$) delineates the solid domain, while the void phase ($\phi(xj) = 0$) corresponds to the void domain. The parameter ξ represents the diffuse interface region, demarcating the transition between these two phases. Following this, the smooth contour is extracted by establishing a value within the design variables plane ($\phi(xj) = 0.5$). To achieve this, the MATLAB function contourf is employed to derive the contour points from the filtered densities distribution data.

Preliminary results: Three numerical examples are explored: the 2D wall, the 3D wall, and the 3D traffic sign. For the 2D wall example, in general, for lower penalty factors, the optimizer prioritizes the removal of the left boundaries, which have higher fluid pressure and shear loading. In this way, less solid material remains in the left region of the design domain. For higher penalty factors, the distribution of solid material showed to be more balanced. Herein, the final compliance values C(x) showed to be lower for higher penalty factor, however, much larger penalty factor will reduce the effects of the interpolation of the coupling condition, which eliminates the information on how to minimize the FSI loading. For the 3D wall example, an optimization grid of 100 x 80 x 80 elements was used (total of 640,000). In contrast, the final fluid-structure system could be modelled using 252,998 tetrahedrons, and 30,038 prisms elements. This demonstrates the advantage of the TOBS-GT method of separating the optimization grid from the FEA software mesh, which allows the meshing of the geometry properly according to the physics, facilitating convergence and better capturing the phenomenon. For the 3D traffic sign, an example with more realistic conditions was explored considering a wind flow of 15 m/s, described as near gale in the Beaufort scale, which generates a Reynolds of 192,000. The structure is designed similarly to an I-beam, including holes that produce a truss-like design. The design of 3D structures via topology optimization considering

FSI is challenging and they are not direct extensions of 2D designs. Finally, the number of elements of the jagged contour geometry and the smoothed geometry is compared. The results shown that the number of elements of the fluid-structure system decreases dramatically by using the smoothing technique.

Preliminary conclusions: The separation of the optimization grid and the FEA mesh ensures the efficient handling of complex fluid-structure interaction (FSI) analyses with distinct governing equations and domains while preserving the core material distribution aspect of conventional topology optimization. This approach involves formulating and solving the optimization problem through sequential integer linear programming using the standard TOBS method, coupled with a geometry trimming process that facilitates CAD modelling of fluid-structure designs. The smoothed contour, akin to a phase field, is derived through a specific technique. These computational components collectively mark a pioneering achievement, as they enable topology optimization to address fluid-structure interaction problems with turbulence models, exemplified by the k-ϵ turbulence model with standard wall functions at fluid and fluid-structure boundaries. Notably, the TOBS-GT method empowers the design of structures under high Reynolds flow loads (up to Re 100,000) for both 2D and 3D scenarios. Future endeavors can extend this approach to tackle nonlinear constraints and more intricate physical phenomena, including compressible flow, rotational flow, and conjugate heat transfer.

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Abstract Title: Virtual Analysis Tools for Enhancing Residence Time and Bubble Characteristics in Fluidized Beds

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Abstract: Adsorption technology, specifically employing fluidized beds in a Temperature Swing Adsorption (TSA) configuration, has emerged as a promising method for reducing CO2 emissions from combustion gases. However, designing large-scale, cost-effective units that minimize environmental impact necessitates carefully considering several variables. Among these, particle residence time and bubble characteristics are two critical factors that significantly influence system efficiency. Particle residence time is of particular importance due to the saturation of solid adsorbent particles over time, necessitating the determination of an optimal residence time within the system. Bubble characteristics, on the other hand, are critical as they influence the heat exchange within the system, a fundamental aspect of the temperature-dependent adsorption process. This study applies virtual analysis tools to optimize these crucial characteristics of fluidized beds for adsorption. A comprehensive Computational Fluid

Dynamics (CFD) model is developed to analyse fluid dynamics and heat transfer within the fluidized bed adsorption stage. This model accurately predicts bubble characteristics using an innovative image recognition algorithm, the results of which have been validated against analytical relations. Additionally, we employ a particle tracing algorithm to evaluate the residence time of each particle, providing a nuanced understanding of particle behaviour within the system. The results obtained from these analyses are presented and discussed, highlighting the significant influence of internal topology on the performance of fluidized beds. These findings underscore the potential benefits of topology optimization for these devices, providing a new pathway for enhancing carbon capture via adsorption. Our research offers valuable insights for developing more effective and efficient large-scale adsorption units, contributing to the global efforts towards a carbon-neutral future.

Keywords: Fluidized Bed, Optimization, Computational Fluid Dynamics, Adsorption, Carbon capture.

Introduction and Objectives: Climate change, primarily driven by anthropogenic carbon dioxide (CO2) emissions, has emerged as one of the most significant challenges of our time. Reducing these emissions is a critical step towards mitigating the impacts of climate change and transitioning towards a more sustainable future. Adsorption technology, specifically employing fluidized beds in a Temperature Swing Adsorption (TSA) configuration, presents a promising method for achieving this goal. However, designing large-scale, cost-effective units that minimize environmental impact involves careful consideration of several variables, including particle residence time and bubble characteristics. These factors significantly influence system efficiency and must be optimized to enhance the performance of the fluidized bed system. This work presents a detailed study that utilizes virtual analysis tools to optimize these crucial characteristics of fluidized beds for adsorption.

Objectives

- Understand and Analyse Critical Variables: The study aims to understand the influence of particle residence time and bubble characteristics on the efficiency of the fluidized bed system. A comprehensive analysis of these variables is undertaken to optimize system performance.

- Develop a Comprehensive CFD Model: One of the primary objectives is to develop a comprehensive Computational Fluid Dynamics (CFD) model to analyse fluid dynamics and heat transfer within the fluidized bed adsorption stage.

- Validate the Image Recognition Algorithm: The study aims to validate the accuracy of an innovative image recognition algorithm used in the CFD model to predict bubble characteristics.
- Evaluate Particle Residence Time: Utilizing a particle tracing algorithm, the study seeks to evaluate the residence time of each particle within the system, providing a nuanced understanding of particle behaviour.

Methodology: The methodology of this study is primarily divided into several stages, each designed to address a specific objective:

1 - Evaluation of Critical Variables: The study begins with a comprehensive examination of the critical variables that influence the efficiency of the fluidized bed system. We specifically focus on particle residence time and bubble characteristics, which are known to impact system performance significantly.
2 - Development of a CFD Model: Following the initial evaluation, we develop a comprehensive Computational Fluid Dynamics (CFD) model. This model is designed to provide detailed insights into the fluid dynamics and heat transfer processes occurring within the fluidized bed adsorption stage.

3 - Application of Image Recognition Algorithm: To predict bubble characteristics accurately, an image recognition algorithm is integrated into the CFD model. This algorithm processes images captured during the fluidization process, identifying and characterizing bubbles based on their size, shape, and distribution.
4 - Validation of the Algorithm: The accuracy of the image recognition algorithm is then validated by comparing its predictions with analytical relations. This validation process ensures the reliability of the bubble characteristics predicted by the CFD model.
5 - Evaluation of Particle Residence Time: In addition to the CFD model, a particle tracing algorithm is employed to evaluate the residence time of each particle within the system. This algorithm tracks the path of individual particles, providing a detailed understanding of their behaviour and interactions within the fluidized bed.
This systematic and comprehensive methodology ensures a robust and nuanced understanding of the factors influencing the performance of fluidized bed systems for adsorption, paving the way for developing more efficient and cost-effective carbon capture technologies.

Preliminary results: Preliminary results from the research provide valuable insights into the performance of fluidized bed systems for adsorption. Analysing particle residence time and bubble characteristics confirms their significant influence on system efficiency, highlighting the potential for enhancing performance by optimizing these variables. The Computational Fluid Dynamics (CFD) model developed for this study provides a detailed understanding of fluid dynamics and heat transfer processes within the fluidized bed. The image recognition algorithm integrated into the CFD model has been validated, demonstrating an accurate prediction of bubble characteristics. Furthermore, the evaluation of particle residence time, conducted using a particle tracing algorithm, reveals a complex interplay of factors influencing particle behaviour and interactions within the fluidized bed. Finally, simulations investigating the influence of internal topology on fluidized bed performance suggest that topology optimization could significantly enhance carbon capture via adsorption. These preliminary results underscore the potential of the approach to contribute to developing more effective carbon capture technologies.

Preliminary conclusions: The importance of particle residence time and bubble characteristics in determining the efficiency of fluidized bed systems for adsorption has been confirmed. This underlines the need for careful optimization of these variables in the design of large-scale units. The Computational Fluid Dynamics (CFD) model provides a robust tool for analysing fluid dynamics and heat transfer processes within the fluidized bed. Moreover, validating the image recognition algorithm integrated into the model ensures the accurate prediction of bubble characteristics. The evaluation of particle residence time using a particle tracing algorithm reveals that internal topology influences the dynamics and characteristics of the fluidized bed. Lastly, as indicated by the simulations, the potential of topology optimization to significantly enhance carbon capture via adsorption points to a promising avenue for future research and development. These conclusions reinforce the research potential for advancing more effective carbon capture technologies.

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Abstract Title: Design Optimization and Experimental Analysis of Supercritical CO2 Centrifugal Compressors

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Abstract: This research project is dedicated to addressing the critical need for innovative solutions to reduce carbon dioxide (CO2) emissions, particularly in the context of oil and gas exploration. The focus of the project is the optimization of centrifugal compressors for Enhanced Oil Recovery (EOR), where CO2 is reinjected into oil wells. The objectives of the project encompass the development of a computational tool for optimizing centrifugal compressors operating under supercritical conditions with pure CO2 and CO2-CH4 mixtures, the design and manufacturing of a test compressor for performance validation, and the construction of an experimental apparatus to characterize compressor performance in "liquid-like" regions near the critical point. The project combines computational modelling, sensitivity analysis, and parametric and topology optimization, pushing the boundaries of knowledge and technology to enhance compressor efficiency, reduce energy consumption, and mitigate emissions. Preliminary results include the implementation of thermodynamic analysis, development of software for real gas property tables, utilization of reduced-order models for flow predictions, 1D and 2D models for preliminary compressor design, 3D fluid-dynamics

simulation of impellers, diffusers and volute, and progress in modelling heat exchangers and structural analysis of compressors. The project's potential impact is substantial, with the ability to reduce CO2 emissions and enhance energy efficiency in carbon capture operations, thus contributing to advancements in the oil and gas industry, energy efficiency, and environmental sustainability.

Keywords: sCO2 centrifugal compressor, design optimization, numerical simulation, experimental analysis

Introduction and Objectives: In our global commitment to reduce carbon emissions, with a particular focus on carbon dioxide (CO2), industries must innovate to capture, utilize, and store this greenhouse gas. In the context of oil and gas exploration, a key strategy is to reinject CO2 into oil wells, a process known as Enhanced Oil Recovery (EOR). The effectiveness of this approach hinges on the performance of centrifugal compressors, which play a pivotal role in elevating the pressure of CO2, often mixed with CH4 (5%), to enable this operation. This process occurs in multiple stages, demanding substantial power and subjecting the gas to supercritical conditions during the final phase. Consequently, any reduction in the energy consumption of the compression system used in carbon capture holds immense potential for diminishing emissions from the overall operation. Therefore, designing a compressor capable of operating efficiently under supercritical conditions with minimal power requirements presents a formidable challenge that pushes the boundaries of our knowledge and technology.
The project has three primary objectives:
1) Develop a computational tool capable of optimizing centrifugal compressors operating under supercritical conditions with pure CO2 and CO2-CH4 mixtures. The optimization process will encompass the entire centrifugal compressor system, including the rotor, vaned diffuser, volute, and will consider fluid-structure interactions. Special attention will be given to operating conditions in the proximity of the "liquid-like" state near the critical point. The goal is to minimize operating costs and reduce environmental impact.2) Design and manufacture a test compressor to assess its performance and validate the computational tool developed in the first objective. The compressor's rotor will be directly driven by a high-speed electric motor, eliminating potential issues associated with gearboxes, high-speed couplings, and seals. Both the compressor and electric motor will be hermetically sealed and immersed in CO2. 3) Develop and construct an experimental apparatus capable of characterizing the performance of the centrifugal compressor prototype under conditions close to the critical point when operating with pure CO2. This apparatus will serve to validate the simulations conducted in the previous phases of the project. It will also facilitate the comparison of different rotor geometries and evaluate the impact of diffuser geometry on compressor performance and its interaction with the rotor. The tests conducted on this apparatus will yield critical data, such as the compressor map, pressure ratio for various flows and rotations, surge conditions, power consumption, and efficiency.

Methodology: The collaboration among our multidisciplinary team has been pivotal in constructing a robust optimization framework for various compression stages. Significant enhancements to existing Computational Fluid Dynamics (CFD) codes have been made, incorporating advanced models to compute thermodynamic properties, simulate turbulent flows with heat transfer, and model fluid-structure interactions in centrifugal compressors handling supercritical gas mixtures. To reduce design variables effectively, sensitivity analysis methods such as Morris, SS-ANOVA, and Fractional Factor Sampling were adapted and utilized. This optimization framework has served to construct accurate response surfaces (utilizing Neural Networks, Kriging, and RBF) for subsequent optimization procedures, including parametric optimization and topological optimization, tailored to achieve the optimal compressor design under diverse operating conditions. Additionally, automating the Equations of State (EoS) for the creation of RGP (Real Gas Properties) tables represents a pivotal and demanding step in realizing the 3D computational modelling of the centrifugal compressor. This project's innovation lies in the optimization of centrifugal compressor designs, accounting for supercritical gas mixtures, fluid-structure interactions, and operation within "liquid-like" regions near the critical point. The scarcity of experimental data in the existing literature, particularly for scenarios involving compressors handling CO2 and CO2-CH4 mixtures under supercritical conditions in "liquid-like" regions, underscores the significance of constructing an experimental apparatus for comprehensive component characterization. This apparatus not only validates our simulations and optimization but also holds great potential for applications, notably Enhanced Oil Recovery (EOR) and Brayton Cycles. To ensure the success of the experimental work, a high-speed electric motor is employed to directly drive the compressor rotor, effectively mitigating potential issues related to gearboxes, high-speed couplings, and seals. Both the compressor and electric motor operate within a hermetically sealed environment immersed in CO2. A high-pressure heat exchanger is utilized to regulate the CO2's temperature at the compressor inlet. The rotor's production incorporates advanced additive manufacturing and micro-machining techniques. Our initial phase involves the operation of the prototype with air to validate the experimental apparatus, measuring instruments, and data acquisition systems. Automation procedures will be developed to create the compressor map and identify the surge condition. Subsequently, the system will be adapted for CO2 operation, integrating a heat exchanger for precise cooling and control of the compressor's inlet conditions. In addition to the demanding centrifugal compressor optimization project, our collaboration with a private company to design a high-speed electric motor capable of functioning under critical conditions positions this development as a substantial innovation for our national industry.

Preliminary results: The project has progressed as planned, with important advances on the various fronts of the project. Regarding the determination of thermodynamic properties, there is no software available that generates real gas property tables (RGP tables) for Computational Fluid Dynamics simulations that include the possibility of carrying out mixture simulations. Both software found, NISTtoRGP (Ansys) and RGPgen (Roger Persky) only allow generating tables for pure substances. Thus, the production of software that generates RGP tables for mixtures represents an important contribution to the CFD simulation of numerous problems

encountered in the Petroleum and Chemical industries. This software must use as a basis the routines of the property calculation software NIST REFPROP and/or CoolPROP, as both use the GERG-2008 equation of state, by Kunz and Wagner (2012). This equation is the most modern currently available for mixtures involving natural gas components. As for the use of reduced order models (low fidelity models), this allows the obtaining of velocity, pressure and temperature fields in internal flows of centrifugal compressors quickly and with low computational cost, regardless of the objective function to be evaluated. It is worth mentioning that such models are efficient for predicting flows in both steady and transient regimes. The proposed reduced order model contributes to a significant reduction in the computational cost of the aerodynamic/fluid-structural optimization process of centrifugal compressors, providing efficient Preliminary designs of turbo machines, including transient phenomena, and can be used to predict compressor performance in real time.

The literature review and Preliminary modelling of an ultra-compact heat exchanger (TCUC) for application in a multi-stage compression system has been carried out according to the activity schedule. The main types of TCUC for the application of this research project were identified and the main geometric characteristics are under computational modelling. The main boundary conditions, as well as numerical solution convergence strategies, were investigated and will be used in the next stages of this project. As for 1D modelling, the optimization of the rotor, diffuser and volute of centrifugal compressors for gas mixtures has been carried out. The modelling developed in the project that preceded the current work has been modified to accommodate the coupling of the rotor, diffuser with *vanes* and the volute. More complex modelling has indicated challenges in modelling convergence and especially due to the interface between the diffuser with vanes and the rotor. Preliminary geometries have been evaluated and subjected to 3D numerical simulation. The next steps are expected to finalize the validation of the 1D tool and move on to coupling it with optimization methods. From the modelling developed by the 1D method, a preliminary compressor has been proposed and 3D computational modelling has been developed. The compressor operating data are those defined for the experimental bench. Manufacturing characteristics of the rotor and diffuser with *vanes* have been taken into consideration when defining the main geometric parameters. A preliminary map of the compressor's behaviour considering different mass flow rates and operating speeds was developed with the aim of identifying possible surge lines, an important characteristic for sizing bearings and bearings. For the next steps, we expect preliminary simulations of the flow in the volute and the submission of the main geometric parameters of the rotor and diffuser with *vanes* to sensitivity analysis and parametric optimization.

preliminary 3D modelling of the centrifugal compressor has been done and mesh density analysis has been completed using the GCI (Grid Convergence Index) methodology. The comparative results between 1D and 3D modelling show that the numerical solution approach is robust and can be considered for the optimization sensitivity analysis steps. The next steps concern the geometric parameterization of the compressor. The implementation of new sensitivity analysis methods has been carried out with the aim of studying methods that can accommodate the optimization characteristics of the centrifugal compressor, which indicate the

possibility of many geometric variables with different operational and constructive restrictions. Methods such as the “Fractional Factor Analysis Method” appear to be promising, as they require few cases to analyse the main effects. The results identified for this method will still be compared with other more traditional methods that reasonably adapt to the characteristics of centrifugal compressors. The next stages of this activity are expected to finalize the implementations and prepare the cases for simulations and definition of the sampling field. During this stage of the project, activities related to the structural modelling of centrifugal compressor rotors were developed with a view to dimensioning stresses, deformations and vibrations/resonance under conditions of fluid-structure interaction (FSI) in a steady state. The results are promising and the project flow under development (*framework)* is being integrated into the multidisciplinary analysis and optimization framework for fluid dynamic sizing aiming for an integrated approach to the project. As for topological optimization, considering incompressible transient IFE analysis, the calculation of the sensitivities of the time compliance integral was implemented with the TOBS-GT method using the COMSOL Multiphysics software as the finite element method solver and the TOBS algorithm as the optimizer. The next steps consist of validating the sensitivities obtained by semi-automatic differentiation with the finite difference method and carrying out the first topological optimization tests in two-dimensional cases. On another point, rotor optimization considering compressible transient IFE analysis is in the implementation phase of a new transient solver within the FEniCS platform TopOpt Foam. The next step is to evaluate the implementation of the transient compressible solver and then move on to the turbulence analysis and identify the vibrations induced by the flow.DAFoam and rhoSimpleFoamTopOpt software for the problem of calculating sensitivity for topological optimization requires special care, especially with regard to the ordering of the result vectors. It is necessary to ensure that the sequence of state variables is the same in both programs so that the comparison can be made correctly. Furthermore, it must be taken into account that DAFoam considers turbulence state variables, while rhoSimpleFoamTopOpt does not, which may result in differences in results. Creating a script that performs the mapping between the two vectors is a solution to the ordering problem, but it is necessary to have knowledge about how the results of the adjoint vector ψ are organized in both programs.Although it is still not possible to calculate the sensitivity correctly using the original code of the rhoSimpleFoamTopOpt, its simplicity and potential justify the efforts made. This code makes it possible to calculate the sensitivity of any type of flow as long as the convergence of the direct problem is obtained and the calculation of residuals is done appropriately. Furthermore, the software uses a platform widely validated by the computational fluid dynamics community (which includes OpenFOAM users) and is easy to understand and the additional implementation is easily parallelizable. Considering topological optimization in fluid-structure interaction problems with restrictions on natural frequencies, to date, part of the proposed objectives has been successfully achieved. The developed computational model allowed the analysis of the forces generated by the flow and the frequency and volume restrictions to improve the impeller design. The topological optimization techniques explored provided efficient solutions for maximizing the stiffness of the impeller subject to natural frequency. However, there is still a lot to be done on this project. It is necessary to explore new

topology optimization techniques, including the possibility of combining different constraints to find even more efficient solutions such as mechanical stress constraints. The implementation of the modal analysis and its sensitivity was carried out in such a way that it is possible to use it with open-source software FEniCS TopOpt Foam (Alonso et al., 2021), and topology optimization tests are being carried out.

Preliminary conclusions: In this project, a sophisticated analysis flowchart is being developed coupling modern computational modelling tools (1D, 2D and 3D) with sensitivity analysis methods, response surface methodology, combined with optimization methods. This procedure will allow the design of centrifugal compressors that can operate with high efficiency and reduced drive power by optimizing this equipment to operate with pure CO2 or with CO2/CH4 mixtures in supercritical conditions. Validation of computational tools requires comparison with experimental tests and due to the scarcity of information in the literature, an experimental bench will be designed and built. The design of centrifugal compressors considering the rotor, diffuser with vanes and the volute is a complex task. The versatility of this flowchart will allow the compression stages to be designed in both the gas -like and liquid -like regions, resulting in an efficient compression system with reduced drive power when compared to conventional designs. Initial studies conducted by the project team indicate that it is possible to reduce the consumption of a typical CO2 compression and capture system on an offshore platform by 9.65%, equivalent to a reduction in CO2 emissions of 1.95 tons per hour. This can be achieved with the last compression stage operating at higher pressures than usual (liquid -like region). Under these conditions, CO2 has a physical behaviour that resembles a liquid, making it possible to reduce the energy consumption of the capture system. An even greater reduction in CO2 emissions is being achieved through optimization of the compressor complete.
The development of structural models for static and dynamic analyses of rotors and centrifugal compressors combined with the context of multidisciplinary optimization involving fluid-structure interaction is a relevant topic for scientific and technological development in the oil and gas area. There are many works in the area related to axial compressors, however for the area of centrifugal compressors in supercritical conditions it is a very scarce topic from a structural point of view with fluid-structure interaction, demanding and justifying research and projects in the area. An important item of this project is the construction of a small-scale compressor prototype that will operate with CO2 under high pressure, a typical condition of the last compression stage used in carbon capture operations. This prototype will aim to collect experimental results to validate the numerical models obtained in the first stage of the project. The construction of an appropriate experimental apparatus for testing, measuring and obtaining data with the prototype is also part of the scope of the project. This new stage also includes the structural and dynamic aspects of the compressor, enabling a complete optimized design of the compressor. As this is a developing technology, we faced several technological challenges throughout the project and two points deserve to be highlighted: (a) technology for cooling high-speed engines – the supercritical carbon dioxide that escapes from the compressor to the engine will be used to cool the electric motor itself. At the same time, its thermophysical and transport properties lead to an increase in the power dissipated by friction within the engine.

The experimental study of this interaction, cooling versus dissipation, will contribute to the development of computational simulation methods by the group and the national company that manufactures the engine; (b) labyrinth joint design technology – the experimental bench will provide data to validate the computational tool under development for labyrinth joint design for high-speed machines. Developing topological optimization of compressible transient flow will allow coupling and improving rotor performance since the optimization can take into account flow-induced vibrations that induce dynamic loads on the structure and cause device wear. These loads must be analysed by fluid-structure interaction and the flexibility of the method will allow generating a rotor design with possible splitters or flow directors that control the dynamic loads generated by flow-induced vibrations. The topological optimization of the impeller considering natural frequency is an area of great scientific and technological relevance, with application in several industrial areas. According to what is currently known, solutions via topological optimization involving natural frequency with geometry cut-off are a scientific novelty. The possibility of developing more efficient impellers can bring numerous benefits, such as increased energy efficiency, reduced costs and less environmental impact. In this context, this project has great potential to contribute to the advancement of science and technology in areas such as energy and the environment.

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Abstract Title: Metamodel-Assisted Structural Design Optimization of CO_2 Centrifugal Compressor

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Abstract: The urgency of carbon emissions reduction emphasizes the pivotal contribution of Carbon Capture, Storage, and Utilization (CCSU) technologies in addressing this global challenge. However, one of the principal impediments to the widespread success of CCSU lies in the substantial energy requirements associated with compression processes. In this context, the design of compressors with optimal aerodynamic and structural efficiency assumes paramount importance. Therefore, the present work presents an application of metamodel-

assisted design optimization tailored specifically to centrifugal compressors, or integrated bladed disks (blisks). Our optimization framework primarily revolves around the reduction of resonance risks while simultaneously ensuring the static structural integrity of blisk components. This is achieved through the incorporation of pre-stressed modal analysis, accounting for inertial loads, centrifugal stiffening, spin-softening, and gyroscopic/Coriolis effects. Objective functions for optimization are based on the Campbell Diagram. The metamodel construction process employs Gaussian Process Regression, with iterative refinement performed by an adaptive Bayesian Sampling methodology. Three distinct optimization algorithms are used: the Genetic Algorithm (GA), Particle Swarm Optimizer (PSO), and the Grey Wolf Optimizer (GWO). To verify the efficacy of our proposed approach, we conduct two comprehensive case studies, including the optimization of a CO_2 centrifugal compressors. Across all cases, our approach yields notable improvements in resonance risk mitigation and overall structural integrity. In the case of the axial blisk, our optimization efforts culminate in the elimination of all resonance conditions, accompanied by a commendable 23% reduction in component mass, while maintaining stress levels akin to the baseline design. For the CO_2 centrifugal compressor (radial blisk), our optimizations result in a significant increase in the bursting margin by 4.31%, and the reduction of critical resonance conditions, thus demonstrating the potential of the approach in enhancing CCSU compression efficiency and reliability.

Keywords: Metamodelling, Structural Optimization, Centrifugal Compressor.

Introduction and Objectives: Centrifugal compressors occupy a pivotal role in optimizing plant efficiency by mitigating potential efficiency losses during the compression process. The existing literature predominantly focuses on the aerodynamic aspects of turbomachinery design due to the significant influence of fluid dynamics and thermodynamics on efficiency. In contrast, limited attention has been given to mechanical design, despite its potential for benefits, such as improved safety, reduced maintenance and material costs, lower power consumption, and extended equipment service life. Therefore, this study's main objective is to implement structural design optimization, with a specific focus on resonance avoidance, one of the most challenging issues in turbomachinery design, especially in integrated bladed disks.

Methodology: The methodology integrates non-linear finite element static stress and modal analyses through a pre-stressed modal analysis approach. It employs Gaussian Process Regression and an adaptive Bayesian sampling method to train metamodels. In the context of optimization, constraints are applied to guarantee the robustness of the optimal design, including safety factors, maximum displacement, and mass considerations. The primary goal of the optimization process is to minimize the risk of resonance, which is achieved using optimization algorithms such as the Genetic Algorithm, Particle Swarm Optimizer, and Grey Wolf Optimizer. To verify the efficacy of our proposed approach two case studies are conducted, including an axial integrated bladed disk (blisk), and a CO_2 centrifugal compressor.

Preliminary results: Across all cases, the optimization yields notable improvements in resonance risk mitigation and overall structural integrity. In the case of the axial blisk, our optimization efforts culminate in the elimination of all resonance conditions, accompanied by a significant 23% reduction in component mass, while maintaining similar stress levels to the baseline design. For the CO_2 centrifugal compressor (radial blisk), the optimizations resulted in an increase in the bursting margin by 4.31%, and a reduction of critical resonance conditions, thus improving the structural integrity of the structure.

Preliminary conclusions: In summary, this study conducted a thorough investigation into the structural design optimization of bladed disk (blisk) and CO_2 centrifugal compressor impellers. Advanced metamodelling techniques and optimization algorithms were employed to systematically explore design variables and obtain optimal outcomes. The primary goal of mitigating structural resonance risk while ensuring structural integrity was successfully achieved. Nevertheless, the research illuminated the intricate nature of resonance avoidance in centrifugal compressors, primarily due to substantial coupling between disk and blade modes.

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Abstract Title: Experimental setup for testing supercritical CO2 centrifugal compressors

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Abstract: The use of supercritical CO2 in EOR (enhanced oil recovery) and as a working fluid in Brayton cycles has been attracting interest due to its high efficiency, compactness, power density, and low operating temperatures. Experimental results for centrifugal compressors are scarce in the literature, even more for the particular case: a compressor working with CO2 at supercritical conditions at the liquid-like region. The objective of this project is to design and build the compressor and an experimental setup to characterize the performance of a centrifugal compressor prototype working with CO2 close to the critical point. The CO2 inside the bench operates in a steady-state cycle. The main components are the compressor - electric motor, expansion valve, and heat exchanger. The installation is for testing the concept of a compressor for supercritical CO2 and surveying the characteristic curves of this machine - relations between pressure ratio, hydraulic power, and efficiency as a function of mass flow and speed. In this

context, the thermodynamic states at the compressor inlet and outlet need to be determined, which means that pressure and temperature (and fluid density at the compressor inlet) are the main variables to be measured.

Keywords: supercritical carbon dioxide, CO2 centrifugal compressor, compressor design

Introduction and Objectives: The use of supercritical CO2 in EOR (enhanced oil recovery) and as a working fluid in Brayton cycles has been attracting interest due to its high efficiency, compactness, power density, and low operating temperatures. Experimental results for centrifugal compressors are scarce in the literature.
The objective of this project is to develop and construct an experimental setup to characterize the performance of a centrifugal compressor prototype working with CO2 close to critical point in the liquid-like region.

Methodology: A steady-state thermo-hydraulic mathematical model is being developed as a support tool for designing the experimental setup. The model includes the calculation of thermodynamic states, compressor power, heat transfer rates, head losses, windage losses and leakage flow (for explanation, see preliminary results). In terms of bench design, some parameters from the SANDIA Labs installation are being used as a reference. At the compressor inlet, the fluid must be in a state close to the critical point, in the liquid-like region. The conditions at the compressor inlet will be close to 7690 kPa and 32 °C. With a pressure ratio of 1.53 and an isentropic efficiency of 0.84; outlet pressure of 11,800 kPa. The design flow of SANDIA was 3.5 kg/s.

Preliminary results: The thermodynamic states at the compressor inlet and outlet need to be determined, which means that pressure and temperature (and fluid density at the compressor inlet) are the main variables to be measured. Starting at the compressor inlet, CO2 is in a state (305 K and 7,690 kPa) close to the critical point. The compressor will raise the fluid pressure to close to 11,800 kPa (pressure ratio of 1.53). The CO2 goes through a thermodynamic cycle, and its state must be brought back to the condition at the compressor inlet. For this purpose, an expansion valve is used to reduce the fluid pressure at the compressor outlet to values close to 7,690 kPa, and a heat exchanger is used to reject heat from the fluid, removing the energy supplied to it by the compressor, closing the cycle. We chose to manufacture a shell-tube heat exchanger, with pressurized CO2 passing through tubes and cooling water passing through the shell. A Coriolis flowmeter is used to measure the compressor inlet mass flow (~3.5 kg/s) and has the additional function of measuring CO2 density. As initially highlighted, thermodynamics states must be determined, therefore pressure and temperature will be measured.
A high-speed electrical motor (50,000 rpm) to drive the centrifugal rotor directly, eliminating potential problems with high-speed coupling and sealing. The compressor and electric motor will share the same hermetic casing and will work immersed in CO2. There will be leakage of CO2 from the compressor into the rotor chamber of the motor; data from SANDIA indicate that this flow rate is around 0.10 kg/s. Labyrinth seals will be used to separate the two compartments

reducing this leakage. This fluid, at high pressure, would result in high windage losses in the engine rotor. Thus, a drainage system for the engine chamber is provided; back-pressure valves will be used to control the pressure inside the motor lower than 20,000 kPa (resulting in a windage loss of about 5 kW; compressor driving power is around 50 kW), the leakage flow is measured using a second Coriolis mass flow meter.
Concerning the auxiliary pieces of equipment, there is a chiller for producing cold water to be supplied to the heat exchanger. There is a vacuum pump for evacuating the line removing air, for later replacement by CO2 - carbon dioxide charging is performed using a positive displacement machine (booster), whose function is to pump liquid CO2 from the tank to the loop. There is a line to purge the system in case of an emergency or normal pressure reduction. System control will be done using a control and data acquisition system.

Preliminary conclusions:
The main difficulty encountered by the team is related to the interaction between the installation and the electric motor (made by a private company). Carbon dioxide leakage from the compressor to the engine is inevitable. At the same time, as it is responsible for windage losses, it serves to internally cool the motor that operates at high speed. Expansion of the fluid through the labyrinth seals will result in a two-phase mixture of CO2 at 250 K. The gas stream must be separated from the liquid, reducing the viscosity of the fluid passing through the engine. We are currently studying how to measure the vapor to liquid ratio and the total mass flow rate. Because lubricating engine bearings involves the use of lubricants that can contaminate CO2, the leak flow must be discarded and liquid CO2 pumped to replace the leak. As the booster used

for this purpose, produces an intermittent flow, we are evaluating the impact of this strategy on the fluctuation of the main flow and thermodynamic states.

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Chairs: Lucy Gomes Sant Anna – Renato Gonçalves

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Abstract Title: Creating an offshore CCS HUB: challenges and opportunities

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Abstract: To reduce greenhouse gas emissions, Carbon Capture and Storage (CCS) is being investigated as a crucial solution due to the urgency of combating climate change. In the Santos Basin, Brazil, characterized by elevated CO2 levels from pre-salt oil extraction, the reinjection of CO2 is imperative. Therefore, CCS technologies offer a pivotal solution, with the integrated CCS HUB concept providing a realistic approach. This research centres on the offshore basins, serving as a case study for the development of technical, regulatory, and socioeconomic models for integrated CCS HUBs. The primary objective is to create an alternative to field decommissioning, ensuring sustained CO2 storage, minimizing closure costs, and enhancing oil production sustainability. By examining diverse aspects of the HUB concept, this research aims to formulate a replicable feasibility protocol, promoting knowledge dissemination for analogous HUB implementations in diverse offshore contexts, aligning with climate change mitigation imperatives.

Keywords: CCS HUB, offshore depleted fields, decarbonization, Brazil.

Introduction and Objectives: The urgent need to manage greenhouse gas (GHG) emissions and establish a low-carbon economy has driven the search for strategies to balance emissions and removals from the Earth's atmosphere. In the Santos Basin, Brazil, known for high CO2 levels associated with oil extraction in the pre-salt area, the reinjection of CO2 is vital. Carbon capture and storage (CCS) technologies are the primary solution, and the concept of an integrated CCS HUB offers a comprehensive approach. This research focuses on the Brazilian offshore basins as a case study to develop technical, regulatory, and socioeconomic models for an integrated CCS HUB. The aim is to create an alternative to decommissioning, ensuring long-term CO2 storage while avoiding costly field closure, ultimately reducing emissions, and improving oil production sustainability. By exploring various facets of the HUB concept, the research seeks to establish a feasibility protocol that can be replicated in similar contexts, facilitating knowledge transfer and the implementation of analogous HUBs. The research effort put out here uses the depleted oil and gas fields as a case study to examine the viability of deploying integrated HUBs for geological storage of CO2 in offshore environments based on technological, regulatory, and socioeconomic modelling. To fully define the deployment of these HUBs, we also want to derive from the oil and gas fields case study an evaluation technique for HUBs that can be used in many scenarios. It will be feasible to determine what are the required elements to create CO2 capture and storage HUBs in various offshore contexts from the development of this protocol, a condition that becomes necessary with the need to mitigate climate change.

Methodology: The proposed methodology for this project comprises three main fronts. The first front focuses on technical modelling and begins with the assessment of geological criteria from existing literature, validating the offshore oil and gas fields reservoirs for CCS suitability. Activities within this front involve data compilation from sources such as ANP technical records, seismic data, well logs, and reservoir data. Criteria from the literature are applied to assess reservoir feasibility and capacity. The second front of the work corresponds to the normative and regulatory studies associated with the project. To comprehend the current state of the art and potential legal gaps that need to be recognized, the first stage of this front involves a review of the law collection on the topic (national and international). Finally, the work's third front includes the socioeconomic components. An integrated vision is needed in the early stages of this front to conduct a preliminary cost estimate. It will be possible to determine the specifications and knowledge gaps needed for a socioeconomic analysis of the offshore CCS Hub.

Preliminary results: Our preliminary findings highlight the significance of developing an integrated CCS HUB in the Santos Basin, specifically focusing on offshore depleted oil and gas fields. Initial assessments demonstrate the technical feasibility of utilizing these reservoirs for long-term CO2 storage, addressing the challenge of high CO2 associated with oil extraction in the pre-salt area. The compilation of geological data, seismic interpretation, and reservoir characterization indicates the potential suitability of these sites. Additionally, we have identified key protocols for assessing the integrity of existing infrastructure, including the fixed platform, pipelines, and wells. These early-stage insights lay the foundation for further research and the establishment of a comprehensive HUB model. On regulatory approach, our results analysis the CCS Bill currently under Brazilian Congress evaluation.

Preliminary conclusions: In conclusion, our preliminary research underscores the promise of the integrated CCS HUB concept as a viable strategy for managing CO2 emissions in the Brazilian offshore basins. The oil and gas fields exhibit encouraging characteristics for geological CO2 storage, and the protocol identified for infrastructure integrity assessment provides a solid framework for future implementation. By leveraging the HUB approach, we can potentially transform mature and depleted oil fields into long-term CO2 storage facilities, reducing emissions and mitigating the environmental impact of oil production. As we continue to work deeper into this project, we anticipate refining our models and feasibility protocols, paving the way for the development of similar HUBs and contributing to a more sustainable energy landscape. Regarding regulatory front, we consider that the CCS Bill will bring legal framework in place to increase credibility for investment.

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Abstract Title: Design Methodology for Gas-Liquid Separators in Methanol Production from CO2

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Abstract: As a sustainable solution to mitigate greenhouse gas emissions while meeting the global demand for energy and chemicals, the production of methanol from carbon dioxide (CO2) has increased attention due to its significant market potential. Methanol is a highly versatile chemical widely used for industrial purposes, such as in gasoline blends, substitute for diesel in heavy-duty vehicles (HDVs), and for its superior quality as a fuel that maximizes engine power. Currently, the methanol market is estimated at $20.4 billion and is expected to grow to $26.6 billion by 2025. The production of methanol through the direct hydrogenation of CO2 can be considered the most established technology for converting CO2 and relies on the use of catalysts based on copper, zinc, and zirconia oxides. Among the processes considered in industrial plants to obtain methanol from the direct hydrogenation of CO2, the separation of the methanol from the gas-liquid mixture plays an important role. It enables the efficient separation of the reaction gas streams from liquid methanol and other byproducts. Thus, gas-liquid separators represent a critical component in the design of pilot plants developed for this purpose, since the fluid that must be separated operates at supercritical conditions. Despite their crucial role, designing gas liquid separators for pilot plants engaged in methanol production from CO2 presents formidable challenges. First, the unique composition of the gas stream, which contains CO2, and potentially impurities, demands innovative separator designs capable of accommodating varying flow rates, pressures, and temperatures. Ensuring high separation efficiency and selectivity pose a technical challenge that necessitates the development of specialized separation techniques. Hence, in this study discusses a methodology for designing gas-liquid separators for this industrial application. The proposed methodology includes determining the geometry based on empirical relations and using a Computational Fluid Dynamics (CFD) technique to evaluate the efficiency of the separation for the designed geometry. Finally, optimization methods are considered to enhance both the geometry and the separation process.

Keywords: Methanol production; Gas-liquid separators; Supercritical conditions; Separation efficiency; Computational Fluid Dynamics (CFD); Geometry determination.

Introduction and Objectives: Global annual carbon dioxide (CO2) consumption currently stands at 230 million tons, valued at nearly US$ 7.7 billion (in 2019 values) [1]. Projections suggest a 3.4% compound annual growth rate in this market until 2027. It's essential to clarify that these figures pertain exclusively to the direct use of CO2 [2]. The environmental benefits

of CO2 transformation are evident, with these products boasting lower CO2 emissions across their lifecycle compared to those derived from fossil fuels [3-5]. However, CO2 conversion faces a substantial challenge due to its high thermodynamic stability, demanding significant energy for its transformation. Thus, efficient catalysts are crucial for this process. Among the various potential CO2 conversion pathways, hydrogenation of CO2 into methanol, methane, or carbon monoxide with heterogeneous catalysts has gained substantial attention. As previously mentioned, methanol is one of the most promising chemicals directly derived from CO2 and can be integrated into various synthesis processes, contributing to a closed carbon cycle. The production of methanol through direct hydrogenation of CO2 is regarded as the most established CO2 conversion technology. It employs catalysts predominantly composed of copper, zinc, and zirconia oxides. Furthermore, laboratory-scale studies have demonstrated high yields in the direct conversion of CO2 into methanol using catalysts made of titanium oxide and rhenium oxide. The next phase in implementing this technology involves scaling up production to a pilot plant with a capacity of 12 Nm3/h. This phase primarily focuses on purifying and recycling the unreacted CO2/H2 mixture. Purification and recycling involve several critical steps. Following this, it encompasses the separation of the gas phase using a gas-liquid separator. The gas phase is efficiently recirculated to the reactor, minimizing waste, while the purified methanol undergoes further refinement through a flash distillation system to attain the necessary purity for commercial use. To determine the appropriate sizing of equipment for the pilot plant and devise an effective methanol separation and purification system, ANSYS Fluent software will be utilized to model the gas-liquid separator. In summary, this work's primary objective is to scale up methanol production, with a particular focus on the purification and recycling stages of the unreacted materials through a gas-liquid separator. Thus a methodology is proposed to determine the required gas-liquid separator design that must separate the liquid methanol from the unreacted CO2/H2 mixture while maintaining process efficiency and stability. This proposed methodology will entail evaluating the gas-liquid separator's ideal geometry, analysing various geometric configurations such as diameter, height, shape, and internal component arrangement to determine the most efficient configuration for component separation.

Methodology: Considering that the main objective is to design a gas-liquid separator capable of handling the specific conditions of the pilot plant to convert CO2 to methanol, the initial step the methodology developed was to construct a Matlab routine that, based on empirical equations, could provide the dimensions of the gas-liquid separator geometry design based on the fluid properties at the inlet of the separator. Since the project is in development, the properties of the mixture which will enter the separator may vary, and thus, using the routine, the gas-liquid separator design can be updated. In the sequence, a Computational Fluid Dynamics (CFD) modelling is applied, considering the geometry obtained from the Matlab routine, to verify the separation efficiency and process stability. Finally, experimental tests will be conducted to validate the gas-liquid separator geometry as well as its connection to the operating conditions of the pilot plant. CFD is a field within fluid mechanics that applies numerical procedures to solve the governing equations of fluid flow. The domain is discretized

into various control volumes, forming the mesh, where the governing equations are solved. Differential equations are discretized into algebraic equations. As a result, the continuous problem is approximated by discrete quantities. In this methodology, the CFD modelling of the gas-liquid separator will allow us to obtain the best optimized geometry for the pilot plant project.

Preliminary results: The Matlab routine, based on empirical equations, has demonstrated its capability to estimate the geometry of the gas-liquid separator. It has successfully provided dimensions that account for variations in fluid properties at the separator's inlet. In addition, CFD modelling, employing the geometry obtained from the Matlab routine, has provided initial insights into the separation efficiency and process stability. Initial simulations suggest that the separator configuration is conducive to efficient gas-liquid separation.

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UFRJ / Amspec

Abstract Title: The Importance of Reservoir Rocks and Fluids Characterization for Ccs Projects: An Experimental Study with Brazilian Rocks and Fluids

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Abstract: The importance of reservoir rocks and fluids characterization for CCS projects has been demonstrated by the execution of an experimental study with Brazilian reservoir rocks and fluids. It has been presented a scenario where the CO2 is injected dissolved in a low salinity brine in an oil reservoir. The work evaluated how the injected CO2 affected reservoir fluids properties and the fluid-fluid and rock-fluid interaction through the measurement of interfacial tension between the fluids and rocks wettability. It has been found the CO2 modifies original reservoir characteristics and the evaluated technique of CO2 injection dissolved in brine is a favourable strategy for CCS projects in the studied system. Additionally, it has been demonstrated that the reservoir characterization is a fundamental stage of CCS projects planning as the CO2 has the potential to change the reservoir in many ways.

Keywords: CCS; Reservoir Characterization, rock-fluid interaction.

Introduction and Objectives: The effort to regulate the CO2 geological storage in Brazil through the law project 1.425/2022 is a movement that follows the world's trends to increase commercial CCS projects. The urgency to expand CCS projects, is happening due to the possibility of making the fossil energy industry more sustainable, as the CO2 geological storage uses the technologies that are already available from the oil and gas industry for more than 50 years. According to CCS Brasil, Brazil has the potential to capture more than 190 million tons of CO2 from very well-identified industrial and energy sources. However, the storage capacity of Brazilian underground reservoirs is not known, which means that it is not well-defined where the captured CO2 would be stored. The measurement of how much CO2 can be permanently stored in geological formations depends on a very detailed reservoir characterization that includes the investigation of the interaction between injected CO2 and the fluids and rocks that are present in each geological formation. Besides the estimation of the storage capacity, the reservoir characterization are also important to understand how the CO2 is going to behave in the reservoir. In other words, reservoir fluids and rocks interaction is a fundamental part of CO2 geological storage because it will offer the key parameters to define the storage capacity, CO2 trapping mechanisms, safety assessment, operational conditions, and monitoring techniques. Also, reservoir characterization reveals the necessary information to define the CO2 injection strategy as it can be done in different ways such as in supercritical state, dissolved into brines, alternated with water, in immiscible conditions, using additives, or many other options. As soon as the CO2 is injected into the reservoir, its contact with reservoir rocks and fluids is going to initiate many different chemical and physical processes that can be favourable or not favourable for CO2 storage. For example, if the CO2 is injected dissolved into a brine, in an oil reservoir, it has the potential to drastically change the rock surface properties such as wettability, while CO2 content also changes the interfacial tension (IFT) between reservoir and injected fluids. These properties are related to the affinity between rock and reservoir fluids and they can determine if CO2 will be retained or flowing between porous media. Aiming to demonstrate the importance of reservoir and fluids characterization and interaction in long term CO2 trapping, this work summarizes one case study that show the effect of CO2 injection on the properties of reservoir fluids, rocks, and their interaction, and how it will impact the performance and efficiency of CCS projects. The fluid-fluid and rock-fluid interactions were studied through IFT and contact angle tests in the function of pressure at 60 °C and the contact angle assays using the Travertine rocks to simulate the carbonate reservoir at 60 °C and 1500 psi.

Methodology: The importance of fluid-fluid and rock-fluid interaction in CCS projects was demonstrated by an experimental study that investigates the rock wettability and IFT changes while the rock is in contact with reservoir oil and injected CO2 dissolved into a brine (carbonated water).

The work was done in 4 steps:

(1) Reservoir fluid samples preparation: reservoir oil and carbonated water have been prepared by the recombination of oil + CO2 and brine + CO2 in the quantities defined by simulations performed in PVTsim software for the reservoir oil sample and OLI studio program for

carbonated water. It was prepared in 2 samples of carbonated water, varying CO2 concentrations in 1.5 and 3.8 % wt., while in the oil the recombination process occurred by transferring 15% wt. of CO2 for oil.
(2) Characterization of prepared samples: experiments to define fluid sample's properties. For the reservoir oil sample, it has been determined, SARA (saturates, aromatics, resins, and asphaltenes) content, total acid number (TAN) and total basic number (TBN) and reservoir pressure densities and viscosities. For carbonated water, it has been determined salinity and pH.
(3) Contact angle and interfacial tension (IFT) tests: the definition of wettability and interfacial tension between reservoir rocks and fluids were performed at a Drop shape analyser (DSA) in the function of pressure at 60 °C using the Travertine rocks to simulate the carbonate reservoir.
(4) Impact of injected carbonated water into rock surface properties: the obtained data has been organized and analysed to evaluate how the carbonated water changes the fluids properties, fluid-fluid and rock-fluid interaction, and how favourable these changes are to keep the CO2 stored into the reservoir.

Preliminary results: Three live fluids were prepared to represent reservoir and injection fluids: reservoir oil (oil + 15% wt. of CO2) and two carbonated waters, being the first one to represent the formation water (brine + 1.5%wt. of CO2) and the second one to represent injection water (lower salinity brine + 3.8 %wt. of CO2). The oil sample has a SARA content of 56% wt. of saturates, 21% wt. of aromatics, 22% wt. of resins and less than 1% wt. of asphaltenes, and TAN of 0.37 mg KOH/g and TBN of 3.79 mg KOH/g., being considered non-acid, despites both TAN and TBN have non-negligible values, indicating the presence of both acid and basic groups in the oil. In addition, the resin and asphaltene contents suggest that oil has effective interfacial-active components. The live oil characterization showed that CO2 presence increased oil density, which was 0.861 g/cm³ for the dead oil while the live oil was 0.875 g/cm³, both performed at 1500 psi and 60 °C. On the other hand, oil viscosity presented an opposite behaviour, decreasing in the presence of CO2, from 10.779 mPa.s in the dead oil to 2.98 mPa.s in the olive oil, in the same conditions of density tests.
The fluid-fluid interaction has been evaluated by the comparison of IFT performed in the two systems: reservoir oil in contact with both carbonated waters. It has been found that the injection water has a higher IFT than formation water, indicating that, for this specific system, the CO2 presence increased IFT. The increasing in IFT is a favourable scenario for CCS once it means the tension between reservoir fluids is increased and the CO2 tends to be trapped into the carbonated water, with reduced interaction with reservoir oil. These results also indicate that IFT is pH-sensitive for oils with considerable TAN, TBN and active compounds, such as asphaltenes and resins.
The rock-fluid interaction has been evaluated by contact angle tests between both carbonated water in contact with travertine rocks. It has been found that the injection water altered the rock's wettability from oil-wet to water-wet. It means, the rock will have a higher affinity with carbonated water than with oil, which is favourable to retain the CO2 stored in the reservoir. This behaviour is related to the interaction of CO2 and the active compounds adsorbed in the rock’s surface.

Due to the changes in oil's densities and viscosities, increasing in IFT and modification of rock wettability, the CO2 injection dissolved into low salinity water, in this scenario, has promoted an easier oil flooding, which is interesting when CCS is combined with oil production (a technique known as enhanced oil recovery – EOR). For this specific scenario, the results indicate that favourable change in the rock wettability happens in low salinity carbonated water, demonstrating that CO2 dissolved into low salinity brine is an interesting strategy to consider while planning a CCS project.

Preliminary conclusions: It has been concluded that investigation of fluid-fluid and rock-fluid interactions between reservoir fluids and rocks and injected CO2 is a key parameter to plan and define CO2 injection strategies for CCS. In the studied system, the CO2 presence affected oil's density and viscosity by increasing density and decreasing viscosity. Also, CO2 increased the IFT and altered the rock's wettability from strongly oil-wet to water-wet. In the presented scenario (CO2 injection dissolved in brines in a carbonate oil reservoir) the observed modification in the live fluid's properties, IFT and rock surface properties were favourable for CO2 storage. However, it is one scenario in multiple options that need to be investigated previously to start CCS projects. This type of reservoir investigation is important to measure how much CO2 can be stored underground and it is also the key to defining the best strategies to inject CO2 in the way to optimize the operation and have the biggest possible amount of CO2 permanently eliminated from the atmosphere. Therefore, reservoir rock and fluids characterization and interaction are a fundamental stage for any CCS project, and it cannot be ignored. The potential to reduce CO2 emissions and even create negative emissions through CCS is enormous, but it demands detailed reservoir rocks and fluids studies. Thus, CO2 changed the interfacial properties of reservoir fluids even as the rock, and analysing this behaviour will allow the best understanding of the system.

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Abstract Title: Evaluation of the influence of the use of different amino acids and superbases in the preparation of deep eutectic solvents for CO2 capture.

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Abstract: The use of DES (Deep eutectic solvents) in the capture of CO2 has been arousing much interest today, mixtures using organic compounds containing alcoholic groups and basic aminos has been presenting good results in processes of absorption of CO2 desorption, recent

studies show that using superbases with amine groups it is possible to deprotonate the alcoholic groups contained in the DESs these react chemically with he CO2 molecules enable a chemical adsorption that can be reverted more efficiently using DES. However, due to the great possibility in the composition of mixtures that produce DES this field needs further studies and better characterization of its properties. This work aims to make a study on the absorption of CO2 by different DES, varying the proportion of HBAs and HBDs in the composition of each DES were produced several mixtures. Bubbling gaseous CO2 up to gas saturation in the mixtures, the solubility of these gases in the produced materials and the influence of different HDAs on the CO2 solubility of the mixtures were studied. The results obtained aim to provide data for future research enabling a better choice of the DES studied in the CO2 capture process.

Keywords: CO2 absorption, deep eutectic solvents, superbase.

Introduction and Objectives: Due to the worsening of climate change every day has been increasing efforts to reduce greenhouse gas emissions, among them CO2 is one of the main responsible for its intensification. One of the most studied alternatives is the capture and storage of CO2, currently this process is costly and made by potentially toxic solvents. Among many pathways studied, deep eutectic solvents (DES) have been arousing a lot of interest, presenting good capacities to absorb CO2 can also promote its capture by chemical and physical interactions. DES are a mixture of a hydrogen donor (HBD) and a hydrogen receiver (HBA) and it is possible to obtain a eutectic mixture with a lower melting point and distinct properties of its pure materials. These have promising properties in processes of capture and separation gases such as CO2, using alcoholic groups HBDs and basic amino as HBAs research has demonstrated have the ability to chemically retain CO2 molecules, using super basic amines it is possible to deprotonate the hydroxyl of alcohols promoting the formation of carbonate groups in DES, promoting chemical adsorption of CO2 molecules. However, these mixtures have some disadvantages, such as high viscosity and high costs in their preparation, requiring further studies aimed at increasing the understanding of their physicochemical properties and the choice in the composition of the most promising DES to capitulate CO2. Thus, this work aims to study the capacity of CO2 capture by several mixtures of DES, focusing on alcohols such as glycerol and other polyols, mixtures were made in various proportions with materials containing groups of basic amines. Using as HDAs some superbases such as DBU, DBN and amino acids containing strongly basic amine groups, mixtures of DES were made in various proportions, the mixtures were characterized and subjected to bubbling with gaseous CO2 until saturation of the material. The results obtained served as a basis to study the CO2 adsorption capacity in the prepared DES, allowing the study of the influence of different amine groups on the molecules used as HDAs, it was also possible to study the influence of the proportion between HDA and HDB in the composition of each DES in the absorption of CO2.

Methodology: In the preparation of the DES, the components were weighed on an analytical balance and mixed in a thermomix at 100ºC to form a homogeneous mixture, following the molar proportion of each HBA HBD for each DES. The resulting mixture was vacuum dried

and stored in a desiccator containing phosphorus pentoxide. For each prepared DES was evaluated its CO2 capture capacity, for this, gaseous CO2 was bubbled until its saturation of the mixture and using an analytical balance was validated the mass difference before and after absorption. The process was interrupted when there was no further difference in the mass of the DES, using the mass difference the amount of CO2 retained in each DES was estimated. The physicochemical properties of DES were also studied using techniques such as DSC, NMR and Karl Fischer.

Preliminary results: Using glycerol and other alcohols such as HBDs were made several mixtures with different HBAs produced the DESs studied. Using compounds containing basic amines, such as superbases and amino acids, several DES with different proportions of HBAs were produced. All mixtures were saturated with gaseous CO2, so it was possible to determine the solubility in mixtures with different super basic amine groups, also, it was possible to study the influence of different proportions of HBAs on the CO2 absorption of the DESs studied.

Preliminary conclusions: It was possible to determine the solubility of CO2 in several DESs, varying the HDAs containing basic amine groups it was possible to study the influence of the use of some superbases and some amino acids containing strongly basic amine groups on the CO2 absorption capacity in different DESs. It was also possible to compare the influence of the proportions of HBAs and HBDs on the capacity of each DES to capture CO2. We gratefully acknowledge the support of the RCGI – Research Centre for Greenhouse Gas Innovation, hosted by the University of São Paulo (USP) and sponsored by FAPESP – São Paulo Research Foundation (2020/15230-5;2014/50279-4) and Shell Brasil, and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&DI levy regulation.

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Abstract Title: Potential of Clay Minerals for CO2 Capture and Storage: Advances from an Atomistic Perspective

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Abstract: The rising levels of atmospheric CO2 have prompted a global push towards devising efficient carbon storage solutions. In this context, the role of clays, which are fine-grained natural materials, emerges as critically significant. Our research comprehensively evaluates clays and their interactions with CO2 at an atomic and molecular level. Using advanced computational methodologies based on the Density Functional Theory (DFT), we examine the layered structures of clays, their inherent charge properties, and their swelling features, all of which influence their CO2 adsorption capacities. Preliminary findings suggest a strong correlation between a clay's interlayered charge properties and its ability to capture CO2. Additionally, specific ions, notably Na and Ni, and their interactions with water molecules are pivotal in this process. Such insights underscore the potential of clays as efficient mediums for carbon storage and pave the way for further innovations in harnessing naturally occurring materials to combat environmental challenges.

Keywords: CO2 capture and storage, clays, experimental, molecular modelling, DFT.

Introduction and Objectives: The exponential rise in atmospheric carbon dioxide (CO2) levels, primarily attributed to anthropogenic activities such as industrial processes, deforestation, and fossil fuel combustion, has become one of our era's most pressing environmental concerns. This escalation in CO2 is directly correlated with rising global temperatures, which subsequently impact various ecological dimensions, including oceanic health, biodiversity, weather patterns, and polar ice melt. Addressing the challenge of curbing and potentially reversing these CO2 emissions is paramount for ensuring a sustainable planetary future. Within the broad spectrum of proposed solutions to this challenge, the sequestration and storage of CO2 stand out as viable approaches. In this context, clays, with their unique attributes, have emerged as promising agents. Clays, integral to many geological and biochemical processes, possess unique composition and structural attributes that make them well-suited for environmental applications, especially in carbon sequestration. Given their widespread presence in the Earth's crust and their natural affinity to interact with a plethora of compounds, clays present a potential scalable solution to the pressing carbon storage challenge. However, to harness this potential effectively, there is a need for a deeper, comprehensive understanding of the intricate interactions between clays and CO2, spanning both macroscopic and atomic scales. Against this backdrop, our research is centred around a dual-fold objective. Firstly, we aim to explore the intrinsic structural and molecular characteristics of smectite-type clays that render them apt for carbon sequestration. Secondly, our focus extends to deciphering the exact dynamics through which clays interact with CO2. This encompasses the nuances of adsorption, the pivotal role of prevalent ions, the critical influence of water molecules, and any resultant structural alterations in the clays during these interactions.

Methodology: Our approach to understanding the intricate interactions between clays and CO2 was a collaborative work evolving computational and experimental methodologies. Density Functional Theory (DFT), based on the quantum mechanical modelling technique, was instrumental in probing smectite-type clays' atomic and molecular interactions with CO2. Through DFT, we could discern clays' electronic configurations and structural properties in the presence of CO2. At the atomic scale, the simulations revealed the orientation of individual atoms within clay layers when exposed to CO2. Also, the adsorption energies, preferred sites of adsorption, and any potential rearrangements at the molecular level. While DFT offered profound theoretical insights, the experimental dimension grounded these insights in tangible reality. Real-world samples of smectite-type clays were carefully prepared and exposed to controlled CO2 environments. Following the CO2 exposure, the clay samples were subjected to a series of tests with advanced spectroscopic and gravimetric experiments. Furthermore, real-time observation techniques were employed to gauge the long-term implications of how clay samples responded to sustained CO2 exposure.

Preliminary results: Our computational explorations with DFT showed that smectite-type clays exhibit a pronounced affinity for CO2 molecule adsorption. These clays' electronic configurations and structural orientations favour CO2 adsorption, leading to significant molecular adhesion. Specifically, the simulations highlighted preferential sites on the clay matrix where CO2 molecules would most likely attach. These sites, often characterised by higher adsorption energies, indicated zones of maximum interaction. The experimental part of our study supported many of the insights gleaned from the DFT simulations, providing tangible validation. Of particular note were the roles prevalent ions, mainly Na and Ni, played in the overall interaction dynamics. Their presence seemed to amplify the clay's affinity for CO2, indicating a synergistic relationship. In scenarios where water molecules were also present, a complex interplay was noticed, with the ions potentially forming nanostructures like nickel hydroxide, further altering the clay’s swelling properties.

Preliminary conclusions: The results from our study present a compelling case for clays as effective mediums for CO2 sequestration and storage. With their distinct structural attributes and molecular affinities, clays offer substantial potential for these applications, showing the critical role of interatomic species and water intermediation in the swelling process.

Allan Cavalari Telles Ferreira
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Abstract Title: Challenges to evaluate CO2 storage potential in Saline Aquifers in Brazil

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Abstract: The development of CCS projects at scale depends on many factors related to the maturity of the institutional environment for decarbonization, as the availability of infrastructure for its entire value chain. One of the key factors is the evaluation of regional CO2 storage potential. Industries and other stationary emitting sources that are the best candidates for adopting carbon capture units in their facilities and even CCS clusters and hubs. Nonetheless, evaluating the country's CO2 storage potential faces relevant barriers. Main properties for classifying a geological context as suitable for CO2 storage include: (i) sufficient depth to ensure the CO2 supercritical phase; (ii) sealing integrity to contain the CO2 within the safety limits, to avoid undesirable migrations; (iii) sufficient storage capacity; (iv) effective petrophysical reservoir properties to ensure that CO2 injection can be economically feasible and that sufficient CO2 can be retained. (Bachu, 2000; Chadwick et al., 2008; IEA-GHG, 2009; Smith et al.,2011; Halland et al., 2011). In practical terms, these properties lead to the following simplified thresholds: (i) 800 meters of depth; (ii) presence of a layer with a low permeability above the reservoir; (iii and iv) adequate combination of porosity, permeability, and thickness. Although it is possible to identify and simplify these thresholds, evaluating even the order of magnitude of the CO2 storage potential in a broader region can be significantly challenging, and many studies end up focusing on depleted oil and gas reservoirs, where it is commonly easier to access data with reasonable quality. Other geological contexts of interest for CO2 storage are often underestimated in the calculations, such as saline aquifers, which usually present a greater storage capacity than depleted oil and gas reservoirs. Publicly available data from wells and seismic studies (ANP, 2023; REATE, 2023) presents reports dated from exploration campaigns, most of them from decades ago, developed with the technology available at that time. These reports comprise annotations, comments, fax, mail, tables and final analysis written by hand, or using a typewriter, providing basic information. Those data were digitalized and published online, but with significant gaps, missing pages, poor calligraphy and, in many cases, notes described as illegible due to their conditions. Therefore, the availability of data from drilled wells and seismic studies is highly concentrated, not covering important territories and often do not present useful information to locate and evaluate saline aquifers. Nevertheless, a complementary source of subsurface data can be found in SIAGAS, a CPRM online platform (SIAGAS, 2023), which provides information from tubular wells drilled for groundwater studies and consumption, although only 4 tubular wells has matched the specifications necessary.

Keywords: CCS, CO2 storage, site screening and exploration, Brazil.

Introduction and Objectives: The development of CCS projects at scale depends on many different factors related to the maturity of the institutional environment for decarbonization, as well as the availability of infrastructure for its entire value chain. One of the key factors is the evaluation of regional CO2 storage potential, which is critical to understand the role of CCS in

emissions reductions for specific regions and countries. By evaluating the total storage capacity and defining the geological contexts to inject CO2, one may analyse the industries and other stationary emitting sources that are the best candidates for adopting carbon capture units in their facilities, as well as the possible transportation networks to allow individual projects and even CCS clusters and hubs.
Brazil is the one of the biggest greenhouse gases contributors, with more than 2.4 billion tonnes of CO2 equivalent emitted in 2021, and around 22% of it was derived from the energy and industrial sectors, great candidates for implementing carbon capture processes (SEEG, 2023).

Methodology: Publicly available data from wells and seismic studies, which consists of reports from exploration campaigns, most of from decades ago, and were developed with the technology available at the time. These reports include annotations, comments, fax, mail, tables, and final analysis written by hand, or using a typewriter, providing basic information (ANP, 2023). Some companies that worked for Petróleo Brasileiro S/A, now Petrobras, from the 1960s to 1990s were required to provide daily technical reports about the activities, expenses, operation progress, and some analysis comparing theoretical information accessible on books, articles, researches about the basin formation and its depth, location, and thickness for example (ANP, 2023). A complementary source of subsurface data can be found in SIAGAS, a CPRM online platform (SIAGAS, 2023), which provides information from tubular wells drilled for groundwater studies and consumption. Analysing and classifying all this data would require manually scraping the files, which would be impractical on a basin scale. For this research, a sample was analysed.

Preliminary results: These data were digitized and published online, but with significant gaps, missing pages, poor calligraphy, and in many cases, notes described as illegible due to their conditions. Therefore, the availability of data from drilled wells and seismic studies is highly concentrated, not covering important territories, and often does not provide useful information for locating and evaluating saline aquifers. An exploratory campaign, bringing together different areas of expertise, should improve the quality and amount of data.

Preliminary conclusions: In conclusion, overcoming the challenges faced in evaluating Brazil's CO2 storage potential in saline aquifers is crucial for the deployment of CCS projects at scale in the country. This requires a comprehensive exploration campaign that identifies the

location, thickness, and pore space of saline aquifers, as well as mature oil and gas reservoirs.

Achieving this will require significant investment, collaboration and coordination among various stakeholders, and the implementation of a regulatory framework for CO2 storage and CO2 pricing mechanisms. By overcoming these challenges, Brazil will be able to play a crucial role in reducing its CO2 emissions and contribute to the global efforts of decarbonization.

Jose Mateo Martinez Saavedra
University of São Paulo

Abstract Title: Studying the kinetics of CO2 hydrogenation into methanol over commercial copper-based catalysts

Authors' Names & Affiliation Institutions of all authors (in order for publication): Jose Mateo Martinez Saavedra, Postdoctoral researcher of University of São Paulo

Abstract: Global climate change is already impacting human environments, and the dire scenario of a 4°C increase in overall global temperatures appears irreversible. In 2023, natural fires and record winter temperatures on Earth serve as evidence of this warming trend, primarily attributed to the continuous rise in atmospheric CO2 levels. Despite efforts to mitigate climate change and implement sustainable technologies in various countries, the international community still faces significant challenges in achieving net-zero emissions goals outlined in the Paris Agreement. One of the most extensively studied strategies for addressing this issue is the conversion of CO2 into methanol. However, the high stability of CO2 presents a significant challenge for the scientific community. Commercial Cu/ZnO/ZrO2 catalysts have garnered considerable attention due to their high selectivity for methanol production and cost-effectiveness. While numerous kinetic studies have been proposed to facilitate the scaling up of this process and its implementation in industries with high CO2 emissions, the true mechanism, and active sites for methanol production within these catalysts remain subjects of ongoing debate among researchers. In this work, we have gathered various kinetics data on CO2 hydrogenation into methanol, which we have used to simulate a reactor for assessing its potential for scaling up the process.

Keywords: CO2 hydrogenation, Simulation, kinetic modelling, Cu catalysts.

Introduction and Objectives: One of the most promising strategies for mitigating carbon emissions is CO2 capture and utilization, as it enables the capture of atmospheric CO2 and its transformation into high-value fuels and chemicals. Methanol is often touted as a future fuel due to its simplicity and lower CO2 emissions when combusted. However, obtaining methanol from CO2 remains a subject of study due to the high chemical stability of CO2, which presents challenges and results in elevated energy costs, ultimately impacting its applicability and sustainability.

Numerous researchers have endeavoured to develop catalytic processes that selectively convert CO2 into methanol at relatively low temperatures and high pressures. Commercially available catalysts like Cu/ZnO/ZrO2/Al2O3 have demonstrated high selectivity for methanol production, making them viable for industrial applications. Extensive research has elucidated the active sites within these catalysts. While pure copper exhibits low methanol selectivity, combining it with metal oxide supports like ZnO or ZrO2 enhances selectivity. For instance, Kattel et al. identified synergistic interactions between Cu and ZnO as the driving force behind catalytic activity for methanol production. Additionally, CuZn nanoclusters exhibit some methanol-favoring characteristics, although to a lesser extent. Previous macrokinetic models have accurately predicted the reactions involved in CO2 hydrogenation to methanol, offering valuable insights for potentially scaling up this process. G. H. Graaf et al. proposed a kinetic model based on the Langmuir-Hinshelwood mechanism, assuming the presence of two active sites on the commercial CuO/ZnO/Al2O3 MK-101 Haldor-Topsoe catalysts. They considered the competitive adsorption of CO and CO2 on the metallic copper site, as well as the competitive adsorption of H2 and H2O on the ZnO oxide site. These two active sites were relevant for temperatures ranging from 210 to 275 °C and pressures between 15 and 50 bar. Similar kinetic models based on the Water Gas Shift reaction have been proposed by Van den Bussche and Froment, Park et al., and Askgaard et al., all focused on the same catalysts but from different suppliers. These models incorporate the presence of CO as a feedstock for the reaction. Notably, the kinetic parameters introduced by Graaf et al. were refined by Jean-François Portha et al. through an optimization modelling process. This work compiles the most studied and relevant macrokinetic models for CO2 hydrogenation into methanol with the aim of simulating chemical reactors tested in the literature and assessing their applicability at an industrial scale.

Methodology: Conduct simulations of kinetic models based on Garaff's work for two and three active sites using commercial Cu-based catalysts. • Develop a kinetic equation based on two active sites that accounts for side reactions through the optimization of kinetic constants. • Perform simulations of the most representative model at an industrial scale. The simulation will be performed using excel and phyton software, and the compressibility factor models for the calculation of thermodynamic properties of reactants and products.

Preliminary results: The first and most representative macrokinetic model in the literature is the work by Graaf et al., which considers two active sites for the hydrogenation of CO2 into methanol. We used the Graaf kinetic model to simulate a non-isothermal adiabatic fixed-bed reactor under the reaction conditions specified in Table 1.
Table 1. Simulation operating conditions

T0-°C 200
P-bar 100
V-mL/min 50

CO2/H2 molar ratio 02:08

Figure 1. Conversion of CO2 during its hydrogenation through a fixed bed over a commercial Cu based catalysts.

Figure 1 displays the conversion profile in relation to the catalyst mass inside the reactor. The graph clearly illustrates that when using small quantities (2-5 g) of catalyst, the conversion rate remains below 5%. However, by increasing the catalyst mass to 10 g, the reactor can achieve a conversion rate of 20%. Beyond this catalyst mass, conversion rates exhibit exponential growth. While this may appear to be a positive outcome, it's important to note that temperature also rises in tandem with conversion. This could pose a challenge, especially considering the system's high pressure and the maximum temperature it can withstand.

Figure 2. Temperature profile through a fixed bed during CO2 hydrogenation reaction over a commercial Cu based catalysts.

Figure 2 illustrates the temperature variations in relation to the catalyst mass. Notably, as the product passes through the 10 g of catalyst, the temperature experiences a significant increase of 120°C. This substantial exothermic reaction underscores the need for precise temperature control.

Figure 3. Producy molar flow evolution through the fixed bed packed with Cu based catalysts.

In Figure 3, we observe the evolution of products across the catalytic bed. It becomes evident that commercial Cu-based catalysts do not exhibit high selectivity toward methanol production. It's crucial to clarify that this initial kinetic model is based on a non-optimized laboratory-scale reactor, which was subsequently enhanced in subsequent years. Therefore, it may not accurately represent the true performance of newly commercialized Cu catalysts.

Preliminary conclusions: The hydrogenation of CO2 into methanol holds substantial potential to align with the sustainability goals outlined in the Paris Agreement, despite several formidable challenges. In this study, we employed a kinetic model proposed by Graaf et al. to simulate a non-isothermal fixed-bed reactor, providing insights into its inner workings. Our findings reveal that the primary challenges to address include the low conversion of CO2 due to its inherent thermodynamic stability and the limited selectivity of catalysts for the desired product. Additionally, the exothermic nature of the reaction presents a significant challenge, necessitating complex cooling systems for the reactor. To gain a more accurate representation of the performance of current Cu-based catalysts available in the market, it is imperative to test and refine the most recent kinetic models.

Leandro Augusto Faustino
Electroactive Materials Laboratory, Institute of Chemistry, University of São Paulo

Abstract Title: Urea electrosynthesis enhanced by localized surface plasmon resonance

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Abstract: Urea production is still conducted using an expensive and harsh method known as the Bosch-Meiser process. Electrocatalytic production offers an advantage and an easier way to synthesize this important product. For this purpose, in this work, a heterojunction of BiVO4/BiFeO3 was mechanically synthesized and decorated with metallic nanoparticles using an ecologically friendly synthesis method. The electrocatalytic properties were enhanced by localized surface plasmon resonance, which was explored in the context of N2 and CO2 reduction. Urea was detected and quantified using 1H NMR and UV-Vis. This work demonstrates how localized surface plasmon resonance can enhance the electrochemical C N coupling at lower overpotentials, thanks to a unique synergism between silver and bismuth nanoparticles.

Keywords: electrocatalysis, N2 reduction, CO2 reduction, urea electrosynthesis, localized surface plasmon resonance.

Introduction and Objectives: Urea is an important chemical feedstock in different areas, especially for the agroindustry. Typically, urea is produced from Bosch-Meiser process. In this process, the CO2 reacts with the NH3 to produce ammonium-carbamate, which is subsequently converted into urea. Although this method is known for its efficiency has drawbacks associated to the high temperature and pressure required. Furthermore, environmental concerns are associated to it, such as greenhouse gas emission. Based on this, the electrochemical C-N coupling under mild conditions seems a good alternative to produce urea. Electrocatalytic production emerges as a superior alternative for synthesizing urea under milder and environmentally friendlier conditions. To promote the electrochemical C-N coupling starting from N2 and CO2, the catalyst must have active sites capable to adsorb both at the same time and near enough. Different approaches have been investigated in order to enhance the adsorption and activation of the gases simultaneously. These approaches include materials with structural defects, like vacancies, materials based on heterojunctions and decoration of oxides with alloys and metallic nanoparticles (NPs). Besides the NPs been used to improve the conductivity and electrocatalytic response, the NPs also exhibit a localized surface plasmon resonance (LSPR) effect. When these NPs are irradiated by a specific wavelength the LSPR effect becomes evident. In this phenomenon, the electromagnetic field of light induces the

electrons on the NPs to oscillate, generating dipoles. Simultaneously, the NPs restore the electromagnetic field to balance the charge in the surface. When both these processes resonate, several effects can be observed, including an increase in the local electric field, localized temperature elevation, and the generation of hot electrons. Based on this, to the best of our knowledge, the electrochemical C-N coupling enhanced by the localized surface plasmon resonance (LSPR) has not been explored to urea yield. Therefore, in this work, a heterojunction of BiVO4/BiFeO3 was synthesized and decorated with silver through mechanochemistry and the electrochemical C-N coupling enhanced by LSPR investigated. In light of these groundbreaking advancements, this study endeavors to showcase the undeniable superiority of electrochemical urea production as the most efficient and eco-friendly approach to meet the growing demands of the modern world.

Methodology: Initially, the catalyst BiVO4/BiFeO3 was synthesized following similar procedures reported in the literature by a wet route. Subsequently, the pristine BiVO4/BiFeO3 material was decorated with silver given Ag@BiVO4/BiFeO3. This process was carried out through a solventless route, mechanochemistry, using a ball milling in the presence of NaBH4 and AgNO3. To gain insights into the milling process, the pristine material was also milled in the presence of NaBH4, that is without silver salt, resulting in M BiVO4/BiFeO3. All the materials were characterized for different techniques, such as, XRD, AAS, SEV, TEM, EDX, XPS, diffuse reflectance and UV-Vis.

Preliminary results: The XRD patterns for all the materials correspond to the patterns for BiVO4 and BiFeO3. In the case of the milled materials, Ag@BiVO4/BiFeO3 and M-BiVO4/BiFeO3, new reflections are observed, indicating the presence of metallic bismuth.
The material's morphology was investigated through SEM. In the case of pristine material, BiVO4/BiFeO3, uniform rice-like structures with sizes around 1 µm were observed. However, for the Ag@BiVO4/BiFeO3, after the milling process, the uniform pattern was lost resulting in small plates with irregular sizes smaller than 1 µm. TEM images of Ag@BiVO4/BiFeO3 revealed the formation of bismuth nanoparticles during the milling process. The EDS results indicated a well-distribution of silver across the material surface. Additionally, other techniques, such as XPS confirmed these observations. The UV-Vis spectra of Ag@BiVO4/BiFeO3 reveal band absorptions at 483 nm and 380 nm corresponding to the plasmon band of bismuth and silver, respectively. Since the milling process can introduce defects into the catalyst structure, the charge carrier density was determined through Mott-Schottky plots. The data indicate that the milling process generates defects in the catalysts structure at least one order of magnitude higher compared to the pristine material. This interesting because it can increase the gases adsorption. The linear sweep voltammetries were carried out in different atmospheres, Ar, N2, CO2 and a mixture of N2 and CO2. It was observed that when the gases were mixed, there was an increasement of current density comparing with other atmospheres. These experiments were also performed under laser irradiation, $\lambda = 455$ nm, which matches with the bismuth plasmon band. Despite under Ar atmosphere, for N2, CO2 and

the mixture of gases were observed an increase in current almost two times higher than observed under dark conditions. Furthermore, the overpotential decreased approximately around 200

mV. Controlled potential electrolysis was carried out under a mixture of N2 and CO2 both in dark and under laser irradiation conditions in order to detect and quantify urea by 1H NMR and colorimetric method. The data revealed that under laser irradiation, the faradaic efficiencies (FE) and urea yield rates achieved were nearly two times higher compared to those obtained under dark conditions. Photoresponse experiments were performed, irradiating at 455 nm for the all the materials, and revealed a synergistic effect between silver and bismuth nanoparticles.

Preliminary conclusions: In conclusion, the successful synthesis and comprehensive characterization of Ag@BiVO4/BiFeO3 have unveiled its remarkable electrochemical prowess in the realm of N2 and CO2 reduction. The mechanical milling process not only yielded metallic nanoparticles but also introduced beneficial defects into the catalyst's structure, enhancing its catalytic activity. Moreover, when submitted to laser irradiation, the electrochemical C-N coupling exhibited significantly improved Faradaic efficiencies and urea yield rates, nearly doubling those achieved under dark conditions. Notably, the unique synergy between silver and bismuth was a standout feature under both N2 and CO2 atmospheres, setting this material apart from its counterparts. Future investigations exploring alternative metallic nanoparticles, such as gold or copper, hold great promise for fine-tuning the electrosynthesis of urea, making this material a prominent choice in the realm of urea production, as previously highlighted.

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0711 – PS8 (TV3) às 17h20	Luís Fernando Nogueira de Sá	Optimizing PEM Fuel Cell Performance with a Pseudo-3D Approach – PS151
0811 – PS10 (TV3) às 10h10	Beethoven Narváez-Romo	Carbon emission reductions in the University of Sao Paulo's transportation – PS196
0811 – PS16 (TV4) às 11h30	Sergio Luciano Avila	Wind turbine diagnostics based on current signatures: a review – PS145
0811 – PS22 (TV2) às 15h20	Antônio Carlos Bastos de Godoi	Cyber Defense System for Smart Grid Communications – PS130
0811 – BECCUS3 (TV2) às 10h10	João Vicotr Vilela Cassiano	Water confined by silica Slits
0911 – BECCUS13 (TV1) às 14h	Paula Barione Perroni	Stainless Steel as Catalyst for Ethanol Oxidation Reaction
0711 – GHG4 (TV4) às 17h20	Daniela Damasceno	Computational Design of Nanostructures and Nanofluidic Systems by Coupling Molecular Simulations with Topology Optimization
0811 – GHG12 (TV4) às 15h20	Caroline Silva Matos	Experimental investigations of Brazilian oxygen carriers for the chemical looping combustion technology: from micro- to macroscale
0911 – GHG20 (TV4) às10h10	Rômulo Luz Cortez	Compressor's Impeller Designs: Topology Optimization for Resonance Mitigation
0911 – GHG23 (TV3) às 14h	Fernanda de Marco	GHG emissions in wastewater treatment plants: nitrous oxide and the importance of data collection and monitoring

SHORT ORAL SESSIONS AWARDS

0711 – CCUS2 (TV2) às 17h20	Fagner Rodrigues Todão	The Role of N-Doped Carbon Structures in the Thermocatalytic CO2 Hydrogenation over Co/SiO2 Catalysts
0811 – CCUSS7 (TV3) às 10h10	Bruna Bacaro Borrego 176	Micractinium sp., mangroves, and biorefineries: A sustainable trio for third-generation ethanol
0811 – CCUS11 (TV3) às 11h30	Vinicio Simizu	Tailoring Pd and Fe Catalysts for Ethanol Synthesis in CO2 Hydrogenation
0711 – NBS1 (TV1) às 17h20	Antonio Yan Viana Lima	Grazing exclusion: a nature-based solution to increase microbial activity in Brazilian desertified drylands
0811 – NBS15 (TV3) às 11h30	José Igor Almeida Castro	Effects of improved pasture and integrated systemas on soil carbon sequestration in Brasil
0811 – NBS17 (TV1) às 15h20	Victória Santos Souza	Nature based solution: cover crops in the Cerrado and their role in greenhouse gas emissions and soil carbon distribution
0811 – SRS5 (TV1) às 10h10	Ricardo Pagio Betini	How can personality influence perception and behavior towards climate change? An exploratory study – SRS104
0911 – CCUS24 (TV4) às 14h	Diego Miranda de Souza Costa	Evaluation of the influence of the use of different amino acids and superbases in the preparation of deep eutectic solvents for CO2 capture
0911 – CCUS18 (TV2) às 10h10	Maitê Gothe	Scale up of a ReOx/TiO2 catalyst for the CO2 hydrogenation to methanol
0811 – CCUS14 (TV2) às 15h20	Lais Borges	Evaluation of intrinsic catalytic activity of rhenium catalysts at CO2 hydrogenation in a fixed bed reactor during a scale-up process

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