Energy Transition
RESEARCH & INNOVATION

SÃO PAULO, 25-27 OCTOBER 2022

Research Centre for
Greenhouse Gas Innovation

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Energy Transition
RESEARCH & INNOVATION

PROGRAM AND BOOK OF ABSTRACTS

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WELCOME TO ETRI 2022

ENERGY TRANSITION RESEARCH AND INNOVATION
SÃO PAULO, 25-27 OCTOBER 2022

After two turbulent years of the COVID-19 pandemic, we are delighted to be able to meet again at ETRI 2022 Energy Transition Research and Innovation at the University of São Paulo, the annual conference of the RCGI Research Centre for Greenhouse gas Innovation.

In addition to the great satisfaction of seeing colleagues again away from the computer screens, the 2022 conference presents the progress of the research underway in the six RCGI programs. We will have 144 papers presented in parallel sessions and posters, in addition to 3 keynote talks, panel discussions and a special moment of innovation on the last day of the event.

Clearly, combating climate change is at the heart of everything that is done at RCGI. But this year, we would like to propose a specific reflection in the wake of the most disruptive years of our generation: How will the efforts to neutralize greenhouse gas emissions be articulated in the midst of adversity, geopolitical instabilities, institutional crises and break of continuity in different aspects of our lives? What are the concrete and immediate steps so that the emission neutrality targets are still achievable?

The goal of achieving a sustainable agenda during the energy transition has not changed. Their boundary conditions have changed. In this context, we invite the scientific and technological community engaged with the topic to debate in yet another ETRI.

You are all very welcome. Enjoy the conference!

Prof. Gustavo R. S. Assi
RCGI Director for Innovation, ETRI Chairman

GENERAL PROGRAM

TUESDAY, 25 OCTOBER 2022

	13:00	**Registration**
OPENING CEREMONY	14:00	**Opening ceremony** Prof. Gustavo Assi, *ETRI Chairman* — RCGI Director for Innovation, University of São Paulo Prof. Julio Meneghini — RCGI Scientific Director, University of São Paulo Dr. Olivier Wambersie — General Manager R&D and Innovation, Shell Prof. Reinaldo Giudici — Dean of Escola Politécnica, University of São Paulo
KEYNOTE TALK	15:00	**Ajay Mehta** Vice President Engineering Technology and Chief Engineer R&D, Shell Group *Getting to Net Zero – Mission Possible*
POSTER SESSION	15:45	**Poster session A** (with coffee break) Choose two presentations to follow from the POSTER PROGRAMME.
PANEL	16:20	**Panel: Technological challenges for energy transition… after "intense turbulence"** **Panelists** Gustavo Assi (moderator) Olivier Wambersie Ajay Mehta Paulo Artaxo Julio Meneghini
CEREMONY	17:20	**ETRI 2022 Excellence Award**
	18:00	**Closing remarks**

GENERAL PROGRAM

WEDNESDAY, 26 OCTOBER 2022

	08:30	**Welcome**
	09:00	**Opening** Welcome and notices
PARALLEL SESSION	09:15	**Parallel session I** *I.1 - Auditorium* *I.2 - Mezzanine room 2* *I.3 - Mezzanine room 3* *I.4 - Mezzanine room 4* Choose your presentations from the PARALLEL SESSIONS PROGRAMME.
POSTER SESSION	10:35	**Poster session B** (with coffee break) Choose two presentations to follow from the POSTER PROGRAMME.
PARALLEL SESSION	11:10	**Parallel session II** *II.1 - Auditorium* *II.2 - Mezzanine room 2* *II.3 - Mezzanine room 3* *II.4 - Mezzanine room 4* Choose your presentations from the PARALLEL SESSIONS PROGRAMME.
	12:30	**LUNCH BREAK**
PARALLEL SESSION	14:30	**Parallel session III** *III.1 - Auditorium* *III.2 - Mezzanine room 2* *III.3 - Mezzanine room 3* *III.4 - Mezzanine room 4* Choose your presentations from the PARALLEL SESSIONS PROGRAMME.
POSTER SESSION	15:50	**Poster session C** (with coffee break) Choose two presentations to follow from the POSTER PROGRAMME.
PARALLEL SESSION	16:25	**Parallel session IV** *IV.1 - Auditorium* *IV.2 - Mezzanine room 2* *IV.3 - Mezzanine room 3* *IV.4 - Mezzanine room 4* Choose your presentations from the PARALLEL SESSIONS PROGRAMME.
	17:45	**Closing remarks**

GENERAL PROGRAM

THURSDAY, 27 OCTOBER 2022

	08:30	**Welcome**
	09:00	**Opening** Welcome and notices
KEYNOTE TALK	09:15	**Carolina Rio** NBS technology leader, Shell *Innovation ecosystems*
INVITED TALKS	09:55	**Innovation from a start-up perspective: cases from Carbonic and Moftech** Maitê Lippel Gothe, Carbonic Dagoberto de Oliveira Silva, Moftech
POSTER SESSION	10:35	**Poster session D** (with coffee break) Choose two presentations to follow from the POSTER PROGRAM.
PANEL	11:10	**Panel: Challenges for high-tech innovation** **Panelists** Gustavo Assi (moderator) Carolina Rio Camila Farias Maitê Gothe Dagoberto Silva Raul Lima
	12:00	**LUNCH BREAK**
PARALLEL SESSION	14:00	**Parallel session V** *V.1 - Auditorium* *V.2 - Mezzanine room 2* *V.3 - Mezzanine room 3* *V.4 - Mezzanine room 4* Choose your presentations from the PARALLEL SESSIONS PROGRAM.
POSTER SESSION	15:40	**Poster session E** (with coffee break) Choose two presentations to follow from the POSTER PROGRAM.
KEYNOTE TALK	16:15	**Paulo Artaxo** University of São Paulo *Where is the "tipping point" for the Amazon Forest?*
	17:00	**Closing ceremony**

PROGRAM OF PARALLEL SESSIONS

PARALLEL SESSION I

I.1 Parallel session I - room 1 (auditorium)

A	Diego Hayashi Alonso	Topology optimization design considering the Wray-Agarwal turbulence model
B	Bruno Souza Carmo	Towards the end of the project STMI: achievements and way forward
C	Jonas Mendonça Targino	An automated approach to generate 2D datasets for seismic data
D	Andre Kubagawa Sato	Estimation of forest fire source term in the Brazilian Amazon

I.2 Parallel session I - room 2 (mezzanine)

A	Bruno Navarro	Impact of the ScRAV1-mediated growth acceleration on sugar accumulation and biomass production of sugarcane
B	Lauana Oliveira e Leandro Oliveira	Strategies to improve the growth and yield of sugarcane plants: amino acids and hormonal profile
C	Marcos Buckeridge	Sugarcane and new bioenergy resources
D	Vitor Favaretto Pinoti	A vector toolbox for CRISPR-mediated genome editing in sugarcane

I.3 Parallel session I - room 3 (mezzanine)

A	Alexandre de Barros Gallo	Using MCDA techniques to organize standardization priorities: The hydrogel case study
B	Alberto J. Fossa	Standardization of Carbon Dioxide Capture, Transportation, Utilization and Storage (CCUS) – Current developments at ABNT and ISO
C	Cylon Liaw	Building a CCUS standardization observatory – First steps towards an insightful tool
D	Renato V. Goncalves	Light-driven Water Splitting to Produce Solar Fuels

I.4 Parallel session I - room 4 (mezzanine)

A	Thaiz da S. Vescovi Chedid	Elaboração de propostas de normalização internacional e serviços de advocacia para implantação e consolidação de marcos legais, regulatórios e de normas para contribuir com os
B	Helen Tatiana Takamitsu	IDENTIFICATION OF TWITTER'S DIGITAL INFLUENCERS ON ENERGY TRANSITION FOR THE DEVELOPMENT OF EFFECTIVE SCIENTIFIC COMMUNICATION STRATEGIES.
C	Karen Louise Mascarenhas	Social Perception and Science Diplomacy on Technology Transitions towards a low carbon society (applications associated with NBS, CCU, GHG and BECCS)
D	Karen Louise Mascarenhas	Key factors of social perception and acceptance of energy low-carbon solutions

PARALLEL SESSION II

II.1 Parallel session II - room 1 (auditorium)

A	Anderson Soares	On the topology optimization of rotor and stator 2D-swirl labyrinth seal design considering forward and backward laminar fluid flow
B	Shahin Ranjbarzadeh	Design of Labyrinth Seals for Carbon Capturing Compressors: Topology Optimization and Experimental Approaches
C	Renato Picelli Sanches	Towards Structural Topology Optimization of Rotating Machinery Considering Fluid-structure Interaction, Turbulence models and 2D-swirl Fluid Flow
D	André Dantas Freire	Baseline and worn labyrinth seals geometry effect on the leakage evaluation using a numerical approach

II.2 Parallel session II - room 2 (mezzanine)

A	Bernardo Lemos	PERFORMANCE OF POLYNOMIAL EXPANSION IN THE DETERMINATION OF THE 2D VECTOR FIELD OF A BUBBLE FLOW IN AN ELECTROLYZER: AN ANALYSIS BY SYNTHETIC IMAGES
B	Alex Marchezini Graça	Protonic conductive electrolytes for high-temperature solid oxide electrochemical cells.
C	Thiago Lopes	Development of an Electrolytic Concentrator of Vinasse
D	Nelson Alexandre Galiote	Electrocatalysts for hydrogen production by ethanol electrochemical reforming

II.3 Parallel session II - room 3 (mezzanine)

A	Heberton Wender	Spontaneous conversion of CO_2 and sulfite to energy using a photocatalytic fuel cell
B	Primaggio Silva Mantovi	Studying Supported Cu & Ag Nanoparticles on 2D MXenes to Enhance C2+ Products at CO2RR
C	Antonio Carlos Roveda Jr.	Electrochemical CO_2 reduction on functional molecule-modified copper surfaces
D	Louise Hase Gracioso	Greenhouse gas-based microalgae bioproducts: A potential biotechnology strategy

II.4 Parallel session II - room 4 (mezzanine)

A	Pedro Brancalion	Restoration of native vegetation for carbon sequestration – Restore.C
B	Maurício Roberto Cherubin	Soil carbon sequestration through integrated agricultural systems in Brazil
C	Chukwudi Nwaogu	Integrated Agricultural Systems: the solution to the global FEES challenges
D	Danielle Mendes Thame Denny	Nature-based solutions: Sustainable development of Latin America

PROGRAM OF PARALLEL SESSIONS

PARALLEL SESSION III

III.1 Parallel session III - room 1 (auditorium)

A	Caetano Rodrigues Miranda	Computational design of nanomaterials by coupling molecular simulations with topology optimization
B	Diego Silva Prado	Topology Optimization for Temperature Swing Adsorption Multi-Staged Fluidized Bed
C	Marcelo Seckler	Post-combustion CO2 capture from biomass flue-gas through adsorption process
D	Helio Henrique Santomo Villanueva	Turbulent oxy-combustion flame stability diluted with CO2

III.2 Parallel session III - room 2 (mezzanine)

A	Felipe Berto Ometto	Green hydrogen production in ethanol-fed SOEC systems
B	Colombo Celso Gaeta Tassinari	CO2 geological storage in Rio Bonito Formation: contribution for negative CO2 emissions through BECCS in southeast Brazil
C	Germano Tremiliosi Filho	Development of materials for hydrogen production via ethanol reform
D	Richardson M. Abraham-A	CO2 storage efficiency considering the sandstone units of the Rio Bonito Formation within southwest São Paulo.

III.3 Parallel session III - room 3 (mezzanine)

A	Dielle Pierotti Procópio	Conversion of CO2 into biopolymers by the regulation of polyhydroxyalkanoates (PHAs) biosynthetic pathway using the photosynthetic cyanobacteria Synechocystis sp.
B	Letícia Oliveira Bispo Cardoso	Unraveling the potential of blue-green algae biomass for bioethanol production
C	Camylle Guimarães Scheliga	BIOPROSPECTION AND IDENTIFICATION OF MICROALGAE FROM MANGROVES AS FEEDSTOCK FOR BIOETHANOL PRODUCTION
D	Antonio C. B. Burtoloso	A new protocol for the synthesis of carbamates and isocyanates from CO2

III.4 Parallel session III - room 4 (mezzanine)

A	Wanderlei Bieluczyk	Greenhouse gas emissions in crop-livestock and crop-livestock-forestry systems in Brazil: a bibliometric analysis
B	Martha Lustosa Carvalho	Nature-based solutions for climate change mitigation: a literature overview
C	Carlos Eduardo Cerri	Improving pasture management as NBS for soil carbon sequestration in Brazil
D	Carlos Eduardo Pelegrino Cerri	Estoque de carbono orgânico do solo (C) em fitofisionomias campestres ou de savana não antropizadas nos biomas do Brasil, uma revisão sistemática de dados publicados

PARALLEL SESSION IV

IV.1 Parallel session IV - room 1 (auditorium)

A	Diana Azevedo	Impact of competitive adsorption of H2O and SO2 on CO2 capture by 13X zeolite
B	Diego Zilli Lima	Numerical structural analyses of centrifugal compressors operating with co2 in a supercritical state
C	Leandro Oliveria Salviano	Design Strategy for Enhanced Oil Recovery Compression Systems Operating with S-CO2
D	Felipe Silva Maffei	Topology optimization of compressible flows using TOBS-GT method

IV.2 Parallel session IV - room 2 (mezzanine)

A	Alexsandro Kirch	The role of water for the CO2 uptake in clays
B	Haline V. Rocha	CO2 geological storage in Rio Bonito Formation coalbeds integrating a BECCS system
C	Jessica Santos Rego	Multiscale modelling of reactive transport and CO2 mineral trapping mechanisms at the Rio Bonito geological formation
D	Bernardo Luiz Harry Diniz Lemos	Recovery of alkali metals using electrodialysis cell: a computer fluid dynamics analysis

IV.3 Parallel session IV - room 3 (mezzanine)

A	Luciano Honorato Chagas	The role of the oxygen vacancies in the isobutene synthesis from ethanol
B	Gabriel L. Catuzo	Catalytic conversion of CO2 to higher alcohols
C	Adolfo Figueredo	CO2 conversion into ethanol using catalyst based on combinations of rhenium and noble metals.
D	Lais Reis Borges	CO2 hydrogenation over Fe oxides catalyst: the effect of pretreatment synthesis on hydrocarbons selectivity

IV.4 Parallel session IV - room 4 (mezzanine)

A	Migue Vera Moreno	A Citizen Science Approach to improving public perception of low carbon society
B	Thiago Brito	Science Diplomacy in the context of Climate Change: a bibliometric analysis
C	Mariana Ciotta	Low-carbon technologies and their association with sustainable development goals
D	Carlos Alberto Labate	Improving the industrial ethanol fermentation using metabolomics and Maldi-TOF

PROGRAM OF PARALLEL SESSIONS

PARALLEL SESSION V

V.1	Parallel session V - room 1 (auditorium)	
A	Paulo Eduardo Batista de Mello	Thermodynamic analysis of multistage carbon dioxide compressor: life cycle condition
B	Wallace Gusmão Ferreira	STRUCTURAL, VIBRATION ANALYSES AND OPTIMIZATION OF CENTRIFUGAL COMPRESSORS FOR SUPERCRITICAL CO2 APPLICATIONS
C	Emilio Carlos Nelli Silva	TOPOLOGY OPTIMIZATION OF COMPRESSIBLE SUBSONIC TURBULENT FLOW CONSIDERING FLUID-STRUCTURE INTERACTION
D	Lucas Oliveira Siqueira	Topology Optimization of Fluid-Structure Interaction Problems Considering Natural Frequency Constraints
E	Nathália Florencia Barros Azeredo	Understanding and optimizing the functioning of selected locally available oxygen carriers for Chemical Looping Combustion (CLC)

V.2	Parallel session V - room 2 (mezzanine)	
A	Rômulo Luz Cortez	Structural Topology Optimization Including Smooth Boundaries Representation
B	Fereshteh Razmara	Topology optimization of non-isothermal PEM fuel cell cathode flow field
C	Dagoberto de Oliveira Silva	MOF's to "Agrotechnology": CO2 Capture and Nutrients delivery
D	Daniel de Carvalho Santos	Computational study of homogeneous catalysts based on non-noble metals in the production of C2+ molecules using CO2 as the primary source of C1.
E	Evandro H.Figueiredo Moura da Silva	Enhancing crop system models for C and N balances: long-term scenarios to improve sustainable agricultural management practices

V.3	Parallel session V - room 3 (mezzanine)	
A	Liane M. Rossi	Introducing the Carbon Capture and Utilization (CCU)-RCGI Programme
B	Maitê Lippel Gothe	Rhenium-based catalysts for the conversion of CO2 to higher alcohols
C	Raphael da Silva Alvim	DFT Simulation of the CO2 Reduction Mechanism on the Mixed-Oxide Catalysts
D	Dyovani Bruno Lima dos Santos	Investigating the perfomance of molybdenum catalysts in the CO2 hydrogenation for higher alcohols production
E	Alvaro Torrez	A machine learning model for adsorption energies of chemical species applied to CO2 electroreduction

V.4	Parallel session V - room 4 (mezzanine)	
A	Matheus Serra de Holanda	Synthesis and characterization of nanostructured materials for application in nanofiltration membranes
B	Andressa Mota-Lima	Electrochemical Technologies for Direct Lithium Extraction from Geothermal Sources and their Industrial Processes
C	Suani Teixeira Coelho	LCA study of the uses of vinasse produced in the sugar-energy sector
D	Suani Teixeira Coelho	CO2 CAPTURE POTENTIAL IN THE SUGAR AND ETHANOL SECTOR IN BRAZIL AND SÃO PAULO STATE
E	Carlos Alberto Martins junior	Molecular Simulations of Boric Acid Filtration by Carbon Structures

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PROGRAM OF POSTER SESSIONS

POSTER SESSION A

A	Poster session A - East Hall		A	Poster session A - West Hall	
1	Vitória Cruz Paluri Piedade	Avaliação do potencial de armazenamento geológico de CO2 na ocorrência de gás de Cuiabá Paulista, Bacia do Paraná, através de modelagem geológica implícita 3D	7	Andre Luis Ferreira Marques	Solar Energy and Data Science: a prediction model for the Amazon Basin
2	Verena M Kaminagakura	Evaluation of microbial fuel cell for electricity generation from niobium-modified electrodes	8	Tiago Valmórbida Dell'Oso Prado	CFD Simulation of a fluidized bed reactor using discrete element method in OpenFOAM
3	Jessenia Brillit Villaverde Herrera	Development of BiVO4 particles with exposed facets to boost light-driven CO2 reduction into solar fuels	9	Diego Miranda de Souza Costa	Development of new Deep Eutectic Solvents (DES) for CO2 capture
4	Luana N. R. Paula	Alcohols Production from CO2 Hydrogenation on Cu-UiO-67 catalysts using H2O as source of hydrogen	10	Ricardo Pagio Betini	What influences public perception of the use of hydrogen as a source of energy?
5	Miguel Ramon Infante Guerra	Synthesis and characterization of heterogeneous catalysts for dimethyl ether production via methanol route.	11	Maria Fernanda Guidi	STATE OF THE ART OF THE SOCIAL PERCEPTION OF RENEWABLE ENERGIES - WIND AND SOLAR
6	Carolina S. Costa	Development of a Catalytic Process for the Conversion of γ-Butyrolactone Into High Added Value Products Using Supercritical CO2	12	Teresa Duarte Lanna	First principles studies of ZIF-67: structural transitions on mesoporous materials for membrane technologies

POSTER SESSION B

B	Poster session B - East Hall		B	Poster session B - West Hall	
1	João B. D. Moreira	Integer linear programming applied to inversion problems in time domain acoustic wave propagation	7	Lucas de Oliveira Bauer	Neural network model for classification of net CO2 fluxes scenarios in the Tapajós Forest, Amazon.
2	Fabiana Matos de Oliveira	Lanthanum strontium-doped manganite modified with nickel for SOFC applications	8	Giovanni Cesar Meira Barboza	Technical and economical feasibility study of the use of Brazilian biomass in chemical looping combustion.
3	Lorenzo K Follador	Effects of CO2 dissolution in electrochemically-relevant Ionic Liquids	9	Gabriel Silveira dos Santos	Functionalized hyperbranched polyglycerols for applications in the capture of CO2 and catalysis.
4	Lucas Duriguettto	CO2 hydrogenation to higher alcohols catalyzed by ReOx/MgO	10	Guilherme Porfirio Baccari	Understanding the Public Perception in CCS literature
5	Luciano Honorato Chagas	The acetic acid synthesis from ethanol and water: The role of Al in the Cu, Zn, Al-based catalyst.	11	Gustavo Chagas de Morais	Citizen Science Approach to the Creation of a Molecularium
6	Elen Maria Feliciano Pereira	Catalytic conversion of short-chain alcohols using CO2 as auxiliary gas	12	Rafael dos Santos Domingues	Separation of Li+/Na+ ions by using nanoestructured materials, polarization and DFT calculations

PROGRAM OF POSTER SESSIONS

POSTER SESSION C

C	Poster session C - East Hall	
1	Jaime Freire de Souza	simwave - A Finite Difference Simulator for Acoustic Waves Propagation
2	Murilo Gomes de Oliveira	Microkinetic Modeling of Ethanol Electro-oxidation Reaction
3	Leonardo Domenico De Angelis	Study of CO2 plasmon-assisted electroreduction over Cu2O-Au nanostructures towards C2 compounds synthesis
4	Bruno Manduca	A metal-organic framework/grafitic carbon nitride composite as photocatalyst for CO2 reduction to methanol
5	Bryan Alberto Laura Larico	Conversion of ethanol to chemicals using rhenium oxide catalysts
6	José Henrique Marques	The influence of the Si/Al ratio on the formation of mesopores in SSZ-13 zeolite by the treatment with NH4HF2

C	Poster session C - West Hall	
7	Itiara Mayra Barbosa de Albuquerque	Adequacy assessment of CO2 satellite measurements for Central Amazonia
8	Giovanni Rodrigues Morselli	CO2 and SO2 Capture by Deep Eutectic Solvents: vibrational spectroscopy and DFT calculations
9	Geraldo Lavigne de Lemos	The methodology developed by the RCGI advocacy group to collect quantitative and qualitative data in climate change themes
10	Celso da Silveira Cachola	State of the art of carbon capture in the industrial sectors: an overview
11	Dindara Silva Galvão	Molecular storytelling on diffusion of low carbon society technologies
12	Bruno José Nagy Antonio	Design and optimization of centrifugal compressors operating with carbon dioxide and mixtures of methane and carbon dioxide

POSTER SESSION D

D	Poster session D - East Hall	
1	Alexandre Olender	Software development for inverse problems in time domain acoustic wave propagation using higher order finite elements
2	Nathália Weber	Rio Bonito Formation suitability for permanent CO2 storage
3	Lázara Hernández Ferrer	"Enhanced electrochemical reduction of N2 with materials of plasmonically active metal nanoparticles, (Au, Ag, Pd, Ru) and (Mo, Ti, Ce), combined with n-type semiconductors."
4	Felipe Machado	Effect of rhenium precursor and composition on the catalytic performance of ReOx/TiO2
5	Fagner Rodrigues Todão	Development of Catalysts for the Direct Conversion of CO2 into Higher Alcohols
6	Lucas Rodrigues da Silva	Synthesis and Characterization of Porous Carbon Materials as Catalysts for CO2 Hydrogenation

D	Poster session D - West Hall	
7	Lucas Neves B S Ribeiro	Experimental validation of labyrinth seals designed by topology optimization
8	Matheus Finamor	Greenhouse gases adsorption in ZIF-8 via first-principle calculations
9	Karen Kristensen Medaglia Motta	What is going on with Carbon Capture and Utilization?
10	Alex Azevedo dos Santos	Atlas of Low-carbon technologies and Hydrogen hubs for the Brazilian Descarbonization
11	Valentina Alzate Rubio	CO2 geological storage opportunity in basalts of the Paraná Basin (Brazil): Perspectives from CO2 mineralization processes in the Serra Geral Formation
12	Gabriela Oliveira	Naphthalenediimide-containing metal-organic frameworks for mixed matrix membranes designed for CO2 separation

PROGRAM OF POSTER SESSIONS

POSTER SESSION E

E	Poster session E - East Hall		E	Poster session E - West Hall	
1	Sabrina Candido Nunes	Evaluation of a microbial fuel cell for the generation of electricity from thermophilic denitrification	7	Julio Cano	Optimization of a thermophilic microbial fuel cell with optimized external resistance
2	Isabella Miranda	Petrography and mineralogy of sandstones from the Rio Bonito Formation, Paraná Basin, as potential for CCS	8	Carlos Alberto Martins Junior	Carbon Nanotubes for CO2/N2 Separation: Insights from Grand Canonical Monte Carlo Simulations
3	Bruna Bacaro Borrego	Bioprospected Microalgae from Mangroves in a Biotechnological Perspective: The Biorefinery Concept	9	Maxiane Cardoso	Brazilian Policies and Legislation for greenhouse gases
4	Vinicio Simizu	Design of catalysts to hydrogenation of carbon dioxide into higher alcohols, such as ethanol, propanol and butanol.	10	Giovana Turquetti	Bioenergy's Social Perception and Its Relevance to Energy Transition
5	Maria Luisa Zardo	Succinic acid production by Bacillus spp. under supercritical CO2	11	Victor Iwao Oliveira Sumikawa	Scaling-up Strategies for Battery-like Electrodes Deployed for Direct Lithium Extraction from Geothermal Sources
6	Diego Sarmento Duncan Lima	Synthesis of MWW and hierarchical lamellar zeolites by mechanical treatment for application in the Methanol to Olefins (MTO) reaction	12	Jacqueline Teixeira Santos	Stability of water nanodroplets: modeling atmospheric phenomena at nanoscale by molecular dynamics

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ABSTRACTS OF PARALLEL SESSIONS

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Topology optimization design considering the Wray-Agarwal turbulence model

Diego Hayashi Alonso - Polytechnic School of the University of São Paulo, USP, SP, Brazil
Juan Sergio Romero Saenz - Federal University of Espírito Santo, ES, Brazil
Renato Picelli - Polytechnic School of the University of São Paulo, USP, SP, Brazil
Emílio Carlos Nelli Silva - Polytechnic School of the University of São Paulo, USP, SP, Brazil

Keywords: Fluid topology optimization; Turbulence; Wray-Agarwal model

Impact: For the design of a supercritical CO2 compressor, we come across one of the current challenges of topology optimization, which is the design of such realistic devices. Therefore, for enabling such type of design, the WA2018 model, which is as accurate as the SST k-ω model, and has advantages in a topology optimization point-of-view, is formulated for topology optimization.

Highlights:
1. The Wray-Agarwal turbulence model (WA2018) is adapted for topology optimization;
2. The TOBS approach, which relies on binary variables solutions, is considered in turbulent flow optimization;
3. A nodal design variable is considered for the TOBS approach, allowing the use of PDE-based pseudo-density filters (such as the Helmholtz filter).

Abstract:
In order to optimize a supercritical CO2 compressor, one highly interesting choice is the use of the topology optimization method, which is the most flexible among the existing optimization methods (parametric, shape, topology). However, making it possible to design industrial or more realistic fluid flow devices is still one of the current challenges in fluid topology optimization. Therefore, it is necessary to consider the turbulence models in more efficient ways inside the topology optimization framework. The most commonly considered approach for modeling turbulent flows in topology optimization is the RANS approach, which is also the least computationally expensive among the other alternatives - such as DNS and LES. However, the RANS models that have been previously considered in topology optimization (Spalart-Allmaras, k-ε, and k-ω models) require the calibration of two additional topology optimization coefficients (normally through a trial-and-error approach). Therefore, here the fluid topology optimization approach is reformulated for the Wray-Agarwal model (WA2018), which incorporates the fluid flow modeling advantages from the k-ε model (freestream modeling) and from the k-ω model (near-wall modeling). It also relies on the solution of a single equation, also does not need the computation of the wall distance. This means that this model requires selecting less topology optimization parameters, while also being computationally less demanding in a topology optimization iterative framework than the previously considered turbulence models in topology optimization. A discrete design variables-based algorithm (TOBS) is considered, which enables achieving clearly defined topologies (solid-fluid) - i.e., where the boundaries are clearly defined during the topology optimization iterations - , while also featuring less dependency with respect to the material model penalization in the optimization process (Souza et al. 2021) and the number of optimization iterations until convergence may be reduced. The traditional pseudo-density material model for fluid topology optimization is considered with a nodal (instead of an element-wise) design variable, which enables the use of a PDE-based pseudo-density filter (Helmholtz filter) together with the TOBS approach. Numerical examples are presented for some turbulent 2D swirl flow configurations for illustrating the approach.

RCGI Project number: 37

Towards the end of the project STMI: achievements and way forward

Bruno Carmo (Poli-USP), Emilio Silva (Poli-USP), Pedro Peixoto (IME-USP), Antoine Laurain (IME-USP), Ernani Volpe (Poli-USP), Rafael Gioria (Poli-USP), Edson Gomi (Poli-USP), Hermes Senger (UFSCar), Eduardo Fancello (UFSC)

Keywords: Seismic inversion; Numerical methods; Geophysics

Impact: The project STMI (Software Technologies for Modelling and Inversion, with applications in seismic imaging) is coming to its end early 2023 and in this presentation we are going to show the main achievements of the team after 4 years of work, and discuss some of the possible ways forward for the research and technology line we initiated within the scope of the other RCGI projects.

Highlights: We will show methods and results for some important aspects of seismic imaging, namely sharp interface identification, absorbing boundary conditions, exponential time-integrators, high-order spatial stencils, cycle skipping mitigation, automatic differentiation, finite-element based FWI, automatic mesh generation, machine learning techniques, applications of topology optimization, level set methods and high performance computing aspects.

Abstract:
The project STMI (Software Technologies for Modelling and Inversion, with applications in seismic imaging) is the only project of the Geophysics programme of the RCGI. It started in mid-2018 and is going to end in early 2023, and in this presentation we will show the main achievements of the project and the possible next steps for the research and technology lines that were initiated in the project. The objectives of the project was to develop software technologies for high performance numerical simulations and to solve inverse problems, which could enable scientists and engineers to develop and test models easier and faster. The key characteristics for the developments are abstraction, automatization, layering, flexibility, portability, performance and integration. The multidisciplinar team was able to dive into techniques and applications that were new to us and give meaningful and solid contributions on many aspects: sharp interface identification, absorbing boundary conditions, exponential time-integrators, high-order spatial stencils, cycle skipping mitigation, automatic differentiation, finite-element based FWI, automatic mesh generation, machine learning techniques, applications of topology optimization, level set methods and high performance computing aspects. We will also discuss the main outcomes of the last annual workshop of the project, which will take place one week before the ETRI2022.

RCGI Project number: 46

An automated approach to generate 2D datasets for seismic data

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Keywords: velocity model; model generator; seismic data;

Impact: The approach allows generating a large amount of samples with a wide variation of features, to train, test and validate results produced by Machine Learning models. In other words, was produced a python code that can use any 2D seismic data, to produce another dataset with N samples, containing variations of layers, salt bodies, faults, and water layer. This large amount of data is crucial to produce good results using Deep Learning techniques.

Highlights: It is proposed a robust, broad, realistic, and parameterizable geological structure model generator using the python programming language. This contributes to fixing the problem related to the scarcity of open seismic data, which is very necessary when developing a technique based on Machine Learning. More specifically use of Deep Learning applied to seismic inversion.

Abstract:
There is a wide range of possible features in geological structures and, for this reason, it is a challenge to model those characteristics. While RTM (Reverse Time Migration) and FWI (Full Waveform Inversion) requires initial guesses as input data and are dependent on model accuracy to speedup calculation and convergence, Neural Networks are complex and non-linear models that usually apply a stochastic gradient descent algorithm that, despite not guaranteed to reach global minima, can produce low error between predicted data and the ground truth, which also allows producing a degree of generalization.

The dependency of local minima in Neural Networks and the accuracy are tightly bounded to sample size in different models and architectures, often being the first of the bottlenecks in network prediction performance.

Modeling a realistic geological structure in a feasible manner is considering most of the characteristics which compose each possible structural feature in geology, although this is not an efficient manner to perform it in order to generate a significant number of models.
A robust, broad, realistic and parameterizable geological structure model generator contributes to fixing one of the first concerns when developing a Neural Network model. In offshore hydrocarbon exploration, some features are commonly found in geological structures related to potential carbonate reservoirs, such as a thick water layer, big salt bodies, geological faults, and complex layered structures.

One of the problems in the seismic area is the scarcity of open seismic data. Considering that in many applications the large amount of information is crucial, as in the case of predictions of seismic data using deep learning techniques.

It is proposed to generate, in an automated manner, an arbitrarily large number of models from an initial velocity model by performing operations that repurpose realistic structures and patterns into a unique combination not present in the original set of samples. This approach is possible by randomly cropping and resizing samples, then adding modeled geological features, e.g. layered structures, salt bodies, faults, water layer, etc. A direct result is to inflate a single 2D sample into unique variations and therefore expand smaller datasets.

In the context of seismic inversion using Machine Learning, it is possible to generate a large amount of samples, to train, test, and validate results produced by Machine Learning models.

Estimation of forest fire source term in the Brazilian Amazon

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Keywords: Source term estimation, Inverse problems, Forest fire

Impact: As the urgency of action to avoid the major consequences of global warming rapidly increases, it is important to improve the tools for a better understanding of greenhouse effect gases sinks and emissions. In this sense, this work contributes to an alternative indirect method for forest fire detection, responsible for a considerable fraction of the Brazilian carbon emission.

Highlights: The work investigated the detection and characterization of forest fires using sensor data from trace gases, using real data from the Amazon region in the experiments. By adopting an adjoint model technique capable of detecting multiple fire focus, which is a common occurrence. The developed algorithm was capable of detecting the fire source using CO and CO2 as tracers.

Abstract:
Global warming is currently one of the most studied topics due to the urgency for a solution. In this regard, understanding the impact of greenhouse gas (GHG) emissions and sinks is of utmost significance. In Brazil, one of the important factors for carbon emissions is forest fires and their relation with deforestation. Therefore, a robust forest fire detection mechanism is essential for analyzing and controlling GHG emissions in Brazil. Currently, fires are mainly detected directly via satellite images, which have a high detection rate. Nevertheless, due to its importance, it is proposed herein an indirect method, to be used in conjunction with the current technic, to improve its efficiency. The proposed methodology is based on the assumption that forest fires can be assumed as a composition of concentrated trace gas or particle emissions, more specifically, of carbon monoxide (CO), carbon dioxide (CO2), and particle matter (aerosols). By detecting the trace gas concentration in some receptors around a fire, the source can be determined by solving an inverse problem, known as source term estimation (STE). The complexity associated with the STE, as an inverse problem, arises from its ill-posed nature, with sporadic, noisy, and sparse input data. Thus, for this work, the objective is to define the parameters of the forest fire, from readings from a finite set of trace gases receptors. The main approaches for the STE problem are adjoint models, optimization techniques, and Bayesian inference, each requiring an atmospheric transport and dispersion (ATD) model. Whereas the two latter methods are interactive, the former reaches the result directly, allowing for a more complex ATD model to be adopted, such as the advection-diffusion. Moreover, it is inherently capable of detecting multiple sources, which is appropriate for situations where multiple forest fires focus occur simultaneously. Therefore, in this work, the adjoint advection-diffusion equation was solved for each receptor to obtain the probability distribution of the source(s) location(s). The experiments used data for the year 2018 in the Brazilian Amazon, considering CO, CO2, and aerosols as tracers. The results showed that a single forest fire focus is detectable using the considered gases as inputs; however, the aerosol data could not reach the same results, as the adopted ATD model is more appropriately applied to gases.

RCGI Project number: 64

Impact of the ScRAV1-mediated growth acceleration on sugar accumulation and biomass production of sugarcane

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Keywords: Bioethanol; Ethylene-responsive factor; Aerenchyma

Impact: The increase in the expression of the ScRAV1 transcription factor led to the acceleration of sugarcane maturation by reaching high sucrose levels faster. This strategy can potentially improve the sugarcane yield by reducing the harvest period.

Highlights: The overexpression of the ethylene-responsive transcription factor ScRAV1 directly affected plant growth, showing a reduction in plant height and biomass, especially in the roots. The transgenic lines showed increased sucrose content in culms. The formation of aerenchyma was delayed in the transgenic lines.

Abstract:
Sugarcane is an essential crop known as a sugar and energy feedstock. The second-generation bioethanol is obtained by the hydrolysis of the cell wall (lignocellulosic residues). It can potentially increase bioethanol production, positively affecting crop productivity without altering planted areas. It is estimated that with sugarcane expansion, Brazilian ethanol can provide a valuable portion of the compensation for carbon dioxide emissions caused by fossil fuels. However, there are still gaps in the comprehension of the cell wall structure, which maintains 1/3 of fermentable sugars that can be used to produce second-generation bioethanol. One of these lacks concerns the regulation of cell wall biosynthesis and degradation processes controlled by the available carbon status in the cells. In this sense, a structure called aerenchyma found in sugarcane roots is characterized by large intercellular spaces in the cortex cells formed by modulation of the cell walls. During aerenchyma formation, cell wall changes are triggered by the ethylene-responsive transcription factor ScRAV1, which negatively regulates the action of an endopolygalacturonase, a pectinase that acts on the middle lamella. Understanding the endogenous hydrolysis processes occurring in the plant cell walls constitutes an excellent strategy for improving the technology for obtaining second-generation bioethanol. Thus, this work aims to elucidate ScRAV1´s role during aerenchyma formation and its impact on the development and maturation of sugarcane. In this way, transgenic plants overexpressing ScRAV1 were evaluated for aerenchyma and culm formation, structural and non-structural carbohydrate contents, biomass proportion, carbon assimilation capacity, and the expression of ScRAV1-target genes. The increased expression of ScRAV1 delayed the root aerenchyma formation, as well as a reduction in the root biomass. Furthermore, more sugars were observed in transgenic lines without modification in the carbon assimilation capacity. We also observed earlier maturation of the plants, which could impact the first-generation bioethanol. This produced proof of the concept that it is possible to increase bioethanol production capacity through the application of knowledge of the mechanisms that control carbohydrate metabolism, which may involve regulating sugarcane aerenchyma formation.

RCGI Project number: 55

Strategies to improve the growth and yield of sugarcane plants: amino acids and hormonal profile

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Keywords: Metabolites. Carbon. Growth.

Impact: Sugarcane bioethanol is a sustainable energy source that contributes to mitigating carbon emissions. During plant development, the interaction of carbon assimilation with amino acids profile and hormonal homeostasis is crucial to increase sugarcane yield. This systemic analysis constitutes a strategy to modulate plant growth and production and adapt to different climatic conditions.

Highlights: Polyamines (PAs) were most abundant in leaves, and putrescine was the central PA. The most abundant amino acids found in the leaves were ornithine and lysine, whereas in culm were asparagine, glutamine, and histidine. The last month of sugarcane development was marked by high levels of hormones indole-3-acetic acid and abscisic acid.

Abstract:
Sugarcane is an essential crop in the agriculture scenario, mainly as a sugar and bioethanol production source. In this sense, attention to the production of biofuels has led to a scientific advance in understanding sugarcane physiology, biochemistry, and molecular biology. Thus, a field experiment that followed the level of carbohydrates and carbon assimilation parameters was analyzed throughout the sugarcane life cycle. Besides carbon flux, changes in hormonal contents and other metabolites are expected during plant development. However, little is known about hormonal and other essential metabolites to modulate plant growth, yield, and adaptation to different climatic conditions. In this study, we measured the content of hormones like polyamines (PAs), indole-3-acetic acid (IAA), and abscisic acid (ABA) and metabolites as amino acids at 1st, 3rd, 6th, and 12th months of development in the field. Distinct metabolite profiles were observed in each organ. PA contents were higher in leaf compared to culm in all months. In both organs, the highest levels were found in the first month. In the leaf, putrescine was the main PA, followed by spermidine and spermine, but this profile was not observed in the culm. During the sugarcane development, the amino acid content was more constant in the leaf than in the culm. The highest levels of ornithine and lysine were found in the leaf, whereas in the culm were asparagine, glutamine, and histidine. The IAA content increased in the leaf after the 3rd month and reached the maximum level in the 12th month. However, culm showed low levels of IAA, except in the third month, which was significantly higher than the leaf. From the third to the sixth month, the content of ABA was similar in both organs. A significant increase in ABA levels was observed at the 12th month in the leaf, whereas no change was observed in the culm. Together, these data provide insights into different hormone and amino acid profiles of leaf and culminating during sugarcane development and pave the way for an integrative understanding of the biological functioning of sugarcane in the field, which can contribute to future strategies to improve yield performance.

RCGI Project number: 55

Sugarcane and new bioenergy resources

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Keywords: Bioethanol; Biomass; Genetic Engineering.

Impact: Increasing sugarcane production without expanding the planted areas could positively impact the carbon footprint, whether in the energy sector or encouraging the consumption of sustainable fuels. This goal can be achieved by obtaining new sugarcane cultivars that reach faster growth or those increasing the developmental traits associated with sugar accumulation.

Highlights: The goals of this project are: (1) Sugarcane genome sequencing at the chromosomal level to increase existing gene mapping. (2) Construction of an expression panel of genes related to sugar signaling. (3) Development of CRISPR/Cas9 protocols for genome editing in sugarcane. (4) Increasing the yield of sugarcane by modifications on growth through different mechanisms such as manipulation of genes involved in carbon partition and growth, changes in hormonal homeostasis, and cell wall modulation. (5) Search for new sources of biomass for bioenergy.

Abstract:
Bioenergy and biomaterials are critical to confronting the effects of climate change. Each country in the world has a different way to contribute with mitigation and adaptation. In the case of Brazil, the production of bioethanol from sugarcane is an outstanding example. The carbon assimilation by photosynthesis, allocated into the biomass, is highly efficient and has allowed the production of more sustainable fuel. However, despite the current efficiency of the sugarcane-ethanol producing system, it is possible to improve it even further. Questions like "can sugarcane plants grow faster?" and "can sugarcane produce more sugar?" are two of the ones we intend to answer in this project. However, those are not easy questions to answer because although the complex trait of sucrose accumulation has been studied extensively in sugarcane, the mechanisms and genetic factors involved in this process are still missing. The absence of an assembled and well-annotated genome database adds an extra layer of difficulty in studies involving sugarcane, which has one of the most complex genomes among plants, with up to eight copies of the same genome in each cell. To overcome these challenges, we proposed goals to achieve the desired traits described above. HiFi and HiC sequencing techniques have been initiated and are expected to generate long genome reading fragments. This strategy will make it possible to obtain complete sequences of the genes themselves and the assembly of genes and their controllers in the genome. This increase in mapping will contribute to the development of genome editing techniques. In order to obtain the genome editing technology for sugarcane, a vector assembly protocol is being established to perform base editing using a gRNA and identify edited sugarcane events tolerant to the herbicide Imazapyr. In parallel, sequences of more than 700 genes were characterized by the construction of a panel of genes related to sugar signaling. The expression values will be obtained in the leaves and culm of sugarcane during different stages of development in plants grown in field conditions. In this experiment, the metabolites that can regulate growth and response to stress, such as amino acids, polyamines, and hormones, were determined. The results showed distinct amino acids, polyamines, and hormonal profiles according to the organ and sugarcane developmental stage. In addition, a transgenic sugarcane line, which showed an acceleration in maturation and high sucrose content, is currently being evaluated, as well as the potential use of new sources for bioenergy. This approach constitutes a complex signaling network associated with the traits that can be modulated,

promoting tolerance and better growth and productivity performance in sugarcane under distinct field conditions.

RCGI Project number: 55

A vector toolbox for CRISPR-mediated genome editing in sugarcane

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Keywords: Sugarcane; Genome editing; CRISPR

Impact: 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. Biotechnology may leverage classical breeding approaches, and CRISPR technologies expanded precise genome editing possibilities. Therefore, establishing an efficient CRISPR-mediated genome editing pipeline would boost sugarcane improvement.

Highlights: Here, 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, we also constructed a set of vectors for straightforward gRNA units cloning by Golden Gate assembly. Altogether, our vector toolbox will facilitate sugarcane genetic analysis research and improvement.

Abstract:
Sugarcane is the source of 80% of the sugar and 26% of the bioethanol produced globally. Accordingly, sugarcane cell wall metabolism, biomass, and stress resistance improvement have been targeted over the last decade. Genetic engineering by CRISPR/Cas9 provides a fast and precise strategy that, combined with classical breeding, will leverage sugarcane improvement. In the present work, we constructed a series of vectors for CRISPR-mediated genome editing in sugarcane by modifying our previously described pGVG vector, which provides high expression levels of foreign genes in this plant species. Initially, the coding sequences (CDSs) of the CRISPR nucleases SpCas9 (Cas9), nSpCas9(D10A)-PmCDA1 (TargetAID), and nSpCas9(H840A)-NC-M-MLV-Delta RNase H (ePPE) were positioned in front of the maize ubiquitin promoter, thus generating the pGVG-Cas9, pGVG-TargetAID and pGVG-ePPE

vectors to be used for classic indel knockout, base editing, and prime editing approaches, respectively. Afterward, the GFP CDS followed by the self-cleaving peptide P2A at its 3' end was cloned in frame with the nucleases N-termini, thus resulting in the pGVG-GFP-Cas9, pGVG-GFP-TargetAID and pGVG-GFP-ePPE vectors, which allows tracking the transgene presence during stable and transient transformation experiments. Lastly, the gateway ccdB-CmR cassette flanked by AttR1 and AttR2 sites was further added to the aforementioned constructs to permit sgRNA expression units cloning through LR reaction. To assemble sgRNA units, we leveraged the Plant Molecular Cloning (MoClo) system based on the Golden Gate assembly method. By executing minor modifications in the MoClo system, we conceived a strategy to assemble sgRNA units under the control of either polymerase II and III promoters also capable to express single or multiple sgRNAs with the tRNA multiplexing approach. Prime editing in plants requires the use of paired prime editing gRNAs (pegRNAs) augmented with repair templates and protective RNA motifs at their 3` end, which often demands difficult cloning procedures. In the present work, we also conceived a simple paired pegRNAs unit cloning strategy by constructing a set of vectors bearing fused RNA motifs and tRNAs sequences thus allowing multiplex assembly by Golden Gate. Furthermore, we deployed the PmeI restriction site in pGVG-Cas9 vector for cloning the homology-directed repair (HDR) template thus adding CRISPR-mediated gene targeting experiments to our portfolio. Collectively, we present a series of vectors that allows fast and facile assembly of genetic constructs for executing simple or complex genetic manipulations by CRISPR/Cas9 in sugarcane.

RCGI Project number: 55

Using MCDA techniques to organize standardization priorities: The hydrogel case study

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Keywords: Hydrogel, MCDA, Standardization

Impact: Technology roadmap-based frameworks are a suitable approach to identifying standardization priorities. However, they usually rely heavily on the expertise of the framework developer. Therefore, MCDA techniques incorporate multiple expert inputs into the framework development. This approach was applied to the Hydrogel Program to develop a set of priorities within a group of standardization topics and standard types.

Highlights: Technology roadmap-based frameworks associated with MCDA techniques allowed incorporating multiple expert inputs to set priorities of standardization topics and standard types. MCDA techniques included in the approach are the Delphi method and Fuzzy-AHP-TOPSIS, involving several survey rounds. The outcomes of this approach applied to the Hydrogel Program are being used in developing a CCUS standardization observatory.

Abstract:
Aiming to identify priorities that could help design a standardization mapping for CCUS standards, an initial investigation of different existing frameworks for standardization was conducted. A technology roadmap-based framework for standardization was considered the approach most suitable. Composed of three strategic dimensions and three tactical dimensions, this technique explicitly characterizes the alignment, coordination, and sequencing of innovation activities (over time). It can be configured to draw out information against other strategic considerations and dimensions.

However, this roadmap-based framework usually relies heavily on the expertise of the framework developer. The use of MCDA techniques is then suggested to incorporate multiple expert inputs toward the decision-making process of developing the framework.

The first strategic dimension (S1 – 'What' innovation activities are relevant to standardization) was analyzed using the Delphi method, including surveys. The second strategic dimension (S2 – 'Why' standardization is needed) and the first tactical dimension (T1 – 'How' to standardize) were analyzed using Fuzzy-AHP-TOPSIS, including new survey rounds. The other two tactical dimensions (T2 – 'Where' standards are developed and T3 – 'Who' is participating) are developed by other activities related to building a CCUS standardization observatory.

The only dimension which will be simplified is the third strategic dimension (S3 – 'When' to be standardized). In general, the framework approach uses concepts of anticipatory, participatory, and responsive standards in a context relative to 'Technology Life-Cycles.' However, the adopted strategy used the results of Fuzzy-AHP-TOPSIS as a prioritization method to decide 'when' to standardize one specific topic before another.

This approach using MCDA techniques in the context of a technology roadmap-based framework for standardization was applied to the Hydrogel Program to develop a set of priorities within a group of

standardization topics and their respective standard types. The outcomes are being used in the development of a CCUS standardization observatory.

RCGI Project number: 47

Standardization of Carbon Dioxide Capture, Transportation, Utilization and Storage (CCUS) – Current developments at ABNT and ISO

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Keywords: CCUS, Standards, Climate Change

Impact: Despite the development of CCU technologies, no standardization environment has been established for discussing CCU standards. The current ISO committee dedicated to CCS could address CCU structurally, while other committees could handle specific CCU issues. Strategic international connections were developed, leading to establishment of a CCUS standardization committee in Brazil.

Highlights: The investigation to determine where CCUS standardization should be conducted led to the conclusion that including CCU in the CCS committee would spare time and reduce the need for experts' mobilization. High-level talks in the Brazilian and ISO standardization environment led to the creation of a Study Commission focused on CCUS under the Environmental Management Brazilian Committee (ABNT/CB-038).

Abstract:
Climate change is a severe threat to present and future generations' development. As a result, Carbon Dioxide Capture, Transportation, Utilization, and Storage (CCUS) has emerged as a tool for mitigating climate change, alongside other programs and strategic decisions such as energy transition, energy efficiency, sustainable behaviors, and so on. There is a need to discuss the peculiarities of CCUS in standards. Particularly determining where CCUS standardization should be conducted and how to establish strategic links between the international standardization environment and Brazilian correlated environments.

ISO/TC 265 is dedicated to CCS and has a working group (WG) for CO2-EOR, a CCU solution. ISO/TC 265 had discussions in the past to examine CCU issues and future actions. If we consider that CCU extends the conventional CCS concept, ISO/TC 265 could adequately address CCU, at least structurally. Where these similarities vary, such as when utilization requirements transcend CCS issues, these subjects can be handled by working groups or subcommittees of other technical organizations. This solution has obvious benefits, particularly sparing the time needed to create a new committee and reducing the need for additional expert mobilization.

There was an absence of specific forums focused on any aspect directly related to CCUS in the national standardization environment. Two pathways to build an international strategic connection were identified: ABNT/CB-038 on Environmental Management and ABNT/CB-116 on Energy Management and Savings. The latter is considered due to its relations with ISO/TMB/CCCC, which have dealt with strategic aspects of international standardization of issues related to climate change, including CCUS.

The initiatives related to ABNT and ISO interface connection through ISO/TC 265 evolved significantly after high-level talks involving the ABNT technical board, which sought to promote the development of new themes associated with climate issues in Brazil. These negotiations led to a decision that monitoring and participation in ISO/TC 265 should be done by a new Study Commission (CE) at ABNT/CB-038. Finally, in June 2022, this commission was formally established (CE-038.007.002 – Captura, Transporte, Utilização e Armazenamento de Dióxido de Carbono), already including the utilization aspects in its scope.

Building a CCUS standardization observatory – First steps towards an insightful tool

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Keywords: CCUS, Standardization, Database

Impact: The CCUS standardization observatory design is based on a technology roadmap-based framework for standardization integrated into strategic and tactical dimensions. In addition to these dimensions, the observatory considers a variety of other standardization data given the audience it can attract. This database wrapped in a user-friendly interface can be an insightful tool to promote CCUS as a climate change mitigation tool.

Highlights: The CCUS standardization observatory considers strategic and tactical dimensions, information regarding who is engaged, abstracts and keywords, stage of development, and others. The observatory may attract a diverse audience, from experts, students, and researchers in CCUS to decision-makers and policymakers interested in climate change issues.

Abstract:
The design of a standardization observatory for CCUS standards was preceded by an initial investigation of different existing frameworks for standardization. In the early 2000s, it was found in the literature developments on standardization frameworks depicting the multiple functions performed by standards. These early frameworks distinguish different aspects involved in standard-making as types of technologies and other innovation activities. However, they are static frameworks and do not answer questions about how standardization should take place over technology development and industry lifecycles. New progress in the following years led to the establishment of frameworks for the standardization processes tackling issues of strategy and tactics. More recent developments consider the knowledge needed to transition between key anticipated innovation activities to predict potential standardization needs for emerging technologies.

The technology roadmap-based standardization framework was considered the most suitable approach for the observatory purpose. Build from the technology roadmap-based framework and integrate standardization's strategic and tactical dimensions. The considered strategic dimensions are: S1 – 'What' innovation activities are relevant to standardization; S2 – 'Why' standardization is needed; S3 – 'When' to be standardized. The tactical dimensions considered are: T1 – 'How' to standardize; T2 – 'Where' standards are developed; T3 – 'Who' is participating.

A specific case study on hydrogel is being developed to answer all strategic and the first tactical dimensions. However, a CCUS standardization observatory could have various new information in addition to the other two tactical dimensions. This is more evident given the diverse audience it can attract, from experts, students, and researchers in the CCUS field, to decision-makers in the CCUS market and policymakers interested in climate change issues.

Therefore, the observatory could handle information regarding how many countries and which ones are engaged in discussing these standards, some brief information about them, including abstracts and keywords, their stage of development, and so on. This database wrapped in a user-friendly interface can be an insightful tool to promote CCUS as a climate change mitigation tool.

Light-driven Water Splitting to Produce Solar Fuels

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Keywords: Green hydrogen, CO2 photoreduction, Artificial Photosynthesis

Impact: Fossil fuels such as coal, oil, and natural gas provide 85% of the world's energy. It is worth emphasizing that an over-reliance on fossil fuels has resulted in an energy crisis, resulting in wreaking havoc on the global economy. Solar-driven water splitting with semiconductor materials is a potential green strategy to simultaneously reduce CO2 emissions and produce renewable fuels, reducing dependence on fossil fuels and thus alleviating the global energy crisis.

Highlights:

- Development of semiconductor-based catalysts to produce environmentally friendly hydrogen.
- Green hydrogen produced by light-driven water splitting.
- Photocatalytic activity is considerably increased by the formation of p-n heterojunctions.
- The RhCrOx cocatalyst inhibits the recombination of photogenerated charges on the surface of SrTiO3.

Abstract:
Renewable energy production from diversified sources (solar, wind, etc.) is essential for the achievement of a sustainable and CO2-free society in a short period of time. Hydrogen is regarded as the most feasible fuel to supply the next generation of fuel cell electric vehicles and associated technologies. Nevertheless, nowadays, hydrogen is mainly produced from fossil fuels by steam reforming of natural gas. In this regard, developing a sustainable and environmentally friendly method of producing hydrogen is essential for a sustainable future. Thus, one of the most promising approaches for producing green and renewable hydrogen is solar-driven water splitting by semiconductor materials acting as photocatalysts. Herein, we have successfully synthesized a class of n-type semiconductor materials (e.g., SrTiO3, BiVO4) as photocatalysts to produce solar fuels by artificial photosynthesis under simulated solar light. Our results show that the materials synthesized in this project have significantly greater photocatalytic activity for hydrogen production than TiO2, which is an important reference material in this reaction. As a strategy to enhance the photocatalytic performance of the single semiconductor materials, co-catalysts were deposited onto the particle surfaces to form a p-n heterojunction, resulting in the photocatalytic improvement. Remarkably, the formation of the heterojunction was responsible for establishing an internal electric field that drives the photogenerated holes into the p-type semiconductor structure, leading to the suppression of electron–hole recombination.

RCGI Project number: 59

Elaboração de propostas de normalização internacional e serviços de advocacia para implantação e consolidação de marcos legais, regulatórios e de normas para contribuir com os compromissos brasileiros vinculados com as NDCs (associados aos temas de Nature Based Solutions – NBS, Carbon Capture and Utilization – CCU, Green House Gases – GHG e Bioenergy with carbono capture and storage – BECCS

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Keywords: BECCS, Normalização, Internacional

Impact: Normalização internacional e serviços de advocacia para implantação e consolidação de marcos legais, regulatórios e de normas para contribuir com os compromissos brasileiros vinculados com as NDCs associado ao tema de Bioenergia com captura e armazenamento de carbono – BECCS.

Highlights: O Brasil ratificou em 2016, através do Congresso Nacional, um documento básico para definir a estratégia de implementação dos compromissos do país a partir de 2020, de acordo com o CNDC (Contribuição Determinada a Nível Nacional). O Brasil espera reduzir as emissões de gases de efeito estufa em 37% abaixo dos níveis de 2005 até 2025, com uma contribuição indicativa subsequente de redução das emissões de gases de efeito estufa em 43% abaixo dos níveis de 2005 até 2030. Para tal, o país comprometeu-se com diversas iniciativas como a aumentar a quota da bioenergia sustentável na sua matriz energética para aproximadamente 18% até 2030, restaurar e reflorestar 12 milhões de hectares de florestas, bem como a atingir uma quota estimada de 45% de energias renováveis na composição da matriz energética em 2030. Neste sentido, o Brasil deve criar um quadro legal e regulamentar, como leis, decretos, portarias, dentre outros documentos. As questões legais e regulamentares são fundamentais para criar uma base para implementar e alcançar os objetivos brasileiros nos CND. Assim, nosso principal objetivo do projeto é analisar e participar dos movimentos internacionais e nacionais em relação às mudancas climáticas, particularmente nos CNDs brasileiros, bem como desenvolver estudos e propostas legais e regulatórias a fim de ajudar o Brasil a implementá-los.

Abstract:
O trabalho pretende analisar as grandes diversidades de legislações, jurisdição de cada país e das instâncias internacionais sobre os temas BECCS. Não existe uma coordenação nem uma definição clara de planejamento estratégico para interação e/ou participação nos movimentos de legislação nacional, incluindo os entes subnacionais, vinculados aos aspectos de mudanças climáticas, particularmente envolvendo BECCS. Considerando a novidade do tema no Brasil, há de se constatar uma ausência de mecanismos legislativos e regulatórios de concretização dos compromissos assumidos perante o Acordo de Paris. Com isso, a problemática relativa ao apoio, construção e efetivamente participação na legislação nacional sobre a temáticas BECCS.

RCGI Project number: 69

IDENTIFICATION OF TWITTER'S DIGITAL INFLUENCERS ON ENERGY TRANSITION FOR THE DEVELOPMENT OF EFFECTIVE SCIENTIFIC COMMUNICATION STRATEGIES.

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Keywords: social network analysis, energy transition, scientific communication

Impact: Moved by climate change mitigation issues and the need to accelerate low carbon energy solutions development, the energy transition has become a hot topic discussed on Twitter, especially by influencers who are shaping the public's perception. Identifying these nods on social media and their narratives is key to generating successful scientific communication strategies.

Highlights: Challenges in promoting energy transition involve successfully communicating knowledge and technology developed by researchers to policymakers and the general public.

- Influencers on social media disseminate narratives about energy transition, including fake news, to a broad range of the public, shaping their perceptions.
- Mastering such processes aims to support scientific communication strategies.

Abstract:
The energy transition has been a hot topic in recent years, both in academia and in the mass media, but it has gained emphasis due to the significant challenges posed by the pandemic, and recently with the rise in the oil price and the energy crisis faced by Europe due to the War of Russia and Ukraine.
This situation generated general apprehension in both the private and public sectors about the world scenario of energy sources and the need to accelerate the ecologically correct and financially viable energy transition, which recovers the economy without compromising the environment, highlighting the importance of the shift to a “green economy” with lower consumption of fossil fuels and reduction of greenhouse gas emissions.
Complex issues such as the energy transition that has many stakeholders involved demand the design of new theoretical and scientific approaches, which cause social impacts in the regions where they are implemented and thus depend on public perception as an key element for the positive receptivity of projects. Therefore, identifying influential people on the subject and supporting the community in understanding the energy transition process through reliable scientific communication, are fundamental items.

The Internet and social networks have enabled new forms of interaction and communication, speeding up the dissemination of information, and generating a huge impact and influence on people's lives. In this scenario, the Digital Influencers emerged, who with their power of persuasion and propagation of information, became strategic people in the communication process in the digital environment.
The objective of the present work was to delimit the network of the most influential nodes on Twitter to detect the main actors and disseminators on the topic of energy transition in Brazil, to identify the rhetoric and arguments used on the topic and combat fake news. For this, data were collected in the official Twitter API. Later, the most influential nodes with the highest degree of centrality were identified, through the analysis of the social networks. The result was the identification of profiles of journalists who deal with the topic of climate change, scientific researchers, politicians, and celebrities, among others. A later phase of the work is a qualitative and detailed analysis of the influencers and the discourse used, thus allowing the delimitation of scientific communication strategies.

RCGI Project number: 70

Social Perception and Science Diplomacy on Technology Transitions towards a low carbon society (applications associated with NBS, CCU, GHG and BECCS)

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Sigmar Malvezzi - Institute of Psychology USP / RCGI

Keywords: social perception, public perception, low-carbon energy solutions

Impact: Innovative social sciences tools and approaches are being developed and applied to identify and understand the social perception of low-carbon energy solutions. Results will contribute with inputs to the decision-making process regarding technology deployment, public policy discussions and communication strategies and narratives.

Highlights: Project 70 approaches social perception through multidisciplinary lenses and perspectives which enrich the research outputs.
- By social perception, we mean to consider the views of all stakeholders: government, policymakers, industry, academia, NGO, media, and the general public.
- It's paramount to keep an open dialogue with all stakeholders aiming for a fair transition.

Abstract:
The social perception was always seen as an essential dimension of various energy issues. However, over the last decades, the energy industry and policymakers, particularly in the O&G industry, perceive that social perception is becoming a much more significant challenge that profoundly affects our energy future. Energy research has been undergoing a major transition from the dominance of physical energy systems to a more challenging energy environment dominated by complex inquiries into the social dimensions of issues. Therefore, the main objective of project 70 is to generate rigorous and innovative scientific knowledge within the field of Social Sciences, aiming at the understanding and mastery of the shaping and change of perceptions, attitudes, resistance, and other subjective features of the Brazilian population on both climate and technology issues for cleaner energy and its development, including NBS, CCU, CHG and BECCS applications. To address such challenging objective, the work is carried out by five workstreams that focus on i) social perception, ii) science diplomacy, iii) socio-historic-geographic data; iv) sociophysics methods, immersive experience, citizen science and art-science; v) innovation and technology transfer. The methodology comprises the articulation of mixed data that is gathered through sets of surveys, interviews, focus groups, and projective and clinical techniques to understand how the totality of variables and their movements are integrated and related to openness and resistance to change. This strategy considers a wide range of variables such as the capillarity of cognitions, values, identities, attitudes, beliefs, perceptions, rituals, prejudice, imaginary, role, and expectations, among others, to be approached under various levels of analyses, such as micro, macro, mezzo, inter, intra groups and strata. It includes the investigation of behaviours and reactions through scenarios and simulations using immersive experiences, and analysis of social media, through data mining and machine learning tools applied to social sciences, using quantitative tools to assess large volumes and diversity of interdependent data, correlating these with socio-historic-geographic data. By applying such methods, the expected results are the identification of relevant social perception features to support decision-making regarding technology, public policy propositions and the development of engaging communication processes.

RCGI Project number: 70

Key factors of social perception and acceptance of energy low-carbon solutions

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Sigmar Malvezzi - Institute of Psychology USP / RCGI

Keywords: social perception and acceptance, public perception, low-carbon energy solutions

Impact: Social acceptance is key for the deployment of big infrastructure projects and low-carbon energy solutions. Therefore, understanding how social perception is formed and modified and which factors influence it is fundamental to engaging different stakeholders in the implementation process.

Highlights:

- This work presents the social perception of many low-carbon energy solutions such as CCUS, bioenergy (without and with CCS – BECCS), hydrogen, solar and wind.
- A criterion was developed through literature review analysis resulting in fifteen factors that influence public and social perception.
- These factors were analysed within each low-carbon energy solutions context and the results aim to support policy development and public engagement.

Abstract:
Social acceptance, which is interpreted as the public active or passive approval of a certain policy, technology or energy solution is a mandatory element of the implementation of energy low-carbon projects. This study aimed to present the main factors that form the perception of different stakeholders, and their acceptance of energy low-carbon solutions such as hydrogen, carbon capture utilization and storage (CCUS), bioenergy with and without carbon capture and storage (BECCS), and renewables as wind and solar. The results, obtained through a review of 535 papers, point out some common factors in low-carbon solutions and show particularities related to each one. To illustrate these factors, our analysis of the social perception of CCS, which was the low-carbon energy solution that represented 40% of the papers in this study, enabled us to classify these factors within fifteen categories: risk perception, benefit perception, psychological factors, technology, previous and actual experience, knowledge, communication, stakeholders, economic aspects, policies, environmental aspects, socio-demographics, cultural aspects, decision-making process, and ethics. Despite particular differences among low-carbon energy solutions, these categories are criteria for deeper analysis. Moreover, the factors detailed within each category enable the identification of variations to be considered, both when analysing the pathways towards energy low-carbon transitions and for structuring the related policies and communication strategies in a specific region.

RCGI Project number: 70

On the topology optimization of rotor and stator 2D-swirl labyrinth seal design considering forward and backward laminar fluid flow

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Keywords: Binary variables, integer linear programming, diodicity

Impact: Uncontrolled carbon dioxide (CO2) emissions can have a great influence on the climate impact. Based on Global Carbon Atlas data emission of CO2 in Brazil increased from 47 to 558 Mt CO2 in the period of 1960 to 2014. Topology optimization of labyrinth seal allows the design of flow path aiming to minimize the gas leakage from compressor to atmosphere by providing innovative interlocking between rotor and stator teeth. Thus, high efficiency seal design can be obtained.

Highlights:

- Stacked-up binary design variables and sensitivities were adopted to provide a proper distinction between rotor and stator components
- Diodicity objective function was expressed in terms of energy dissipation and vorticity
- The interlocking teeth direction between rotor and stator is favored by the modelling strategy
- The continuation approach was suitable for full fluid domain initial guess
- Geometry trimming improved the diodicity predicted by porous solid model

Abstract:
In the quest to reduce the climate effects caused by CO2 emissions, the improvement of the liquid-gas labyrinth seals designs leads the interest of industries to reduce the gas leakage. Literature usually adopts fluid flow shape optimization as the main tool to improve the design of these mechanical devices. However, this problem is three-dimensional by nature which increases the computational cost of simulation and, consequently, for the optimization. Another challenge is the fact that both rotor and stator walls need to be tracked (since both have distinct angular speed) and a minimum distance should be maintained between both solid phases. In this work, we employ a two-step optimization methodology by using the Standard TOBS and the TOBS-GT (Topology Optimization of Binary Structures with Geometry Trimming) method to solve a 2D axisymmetric seal problem considering two distinct rotational velocities on solid material. We maximize the diodicity by minimizing the forward energy dissipation while maximizing the backward vorticity subjected to a fluid volume constraint. The 2D swirl flow is governed by the Navier-Stokes equations in the inertial reference frame. The governing equations are solved via the Finite Element Method considering axisymmetry and the optimization problem is solved by using sequential integer linear programming. In order to avoid jagged geometries, which affects the accuracy of flow modelling, we adopt an additional step to create a smooth wall representation. The numerical example shall elucidate how the solid (by considering a porous medium or trimming out of the analysis) modelling influences the topology evolution. We assumed real CO2 gas properties and realistic dimensions for the seal. Finally, our method predicted that porous material model favors radial interlocking teeth on seal, while trimming procedure improved the diodicity by

redistributing solid material to an axial labyrinth. Therefore, TOBS and TOBS-GT shows to be an improved method for binary seal design.

RCGI Project number: 65

Design of Labyrinth Seals for Carbon Capturing Compressors: Topology Optimization and Experimental Approaches

Shahin Ranjbarzadeh, Renato Picelli, Fernando Pinto, Julio Meneghini, EMilio Carlos Nelli Silva

Keywords: Labyinth Seal, Topology optimization, Carbon dioxide

Impact: Recently, reduction of Greenhouse Gases (GHG) emissions attracts much attention and can have a significant impact on climate change. Leakage of carbon dioxide and methane from labyrinth seal in turbo-machinery devices such as compressors and turbines is one of the sources of GHG emission to the atmosphere. Labyrinth seals are the oldest and the most famous mechanical sealing solution in the industry and play a vital role in preventing and reducing GHG emission. Topology optimization is an optimization method that distributes material inside a design domain to find the optimized topology of a structure based on a specified objective function and constraints.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 an optimized design with the highest efficiency and less leakage.

Highlights:

Recently, reduction of Greenhouse Gases (GHG) emissions attracts much attention and can have a significant impact on climate change.

Labyrinth seals are the oldest and the most famous mechanical sealing solution in the industry and play a vital role in preventing and reducing GHG emission.

optimized designs obtained by topology optimization demonstrate a leakage reduction up to 54% and experimental test results confirmed the numerical simulations.

Abstract:
Recently, reduction of Greenhouse Gases (GHG) emissions attracts much attention and can have a significant impact on climate change. Leakage of carbon dioxide and methane from labyrinth seal in turbo-machinery devices such as compressors and turbines is one of the sources of GHG emission to the atmosphere. Labyrinth seals are the oldest and the most famous mechanical sealing solution in the industry and play a vital role in preventing and reducing GHG emission. Topology optimization is an optimization method that distributes material inside a design domain to find the optimized topology of a structure based on a specified objective function and constraints.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 an optimized design with the highest efficiency and less leakage. During the last decade, advancement of Topology Optimization (TO) join with Additive Manufacturing (AM) shows a potential in design and the improvement of the fluidic devices such as pumps and valves. Thus, this paper presents a topology optimization approach for designing the labyrinth seals for carbon dioxide compressors with operational rotation speed up to 4000 rpm with application in carbon capturing and storage system. Later, optimized prototypes is fabricated via additive manufacturing using 3D polymer printer. Finally, for validation of numerical results, experiment is carried out utilizing a test rig of labyrinth seal. The model is developed based on the low Reynolds steady-state Navier-Stokes equation and considers an axisymmetric flow with flow rotation around the shaft (2D swirl flow model). Diodicity of dissipation energy is defined as an objective function to reduce the methane leakage. Several numerical examples is carried out to investigate and demonstrate the effectiveness of the optimization procedure. Despite assuming low Reynolds number

formulation in topology optimization, results are in good agreement with CFD and optimization of labyrinth seal considering turbulent flow in the literature specially in which concerns the inclination of teeth toward the inlet. Furthermore, optimized designs obtained by topology optimization demonstrate a leakage reduction up to 54% and experimental test results confirmed the numerical simulations.

RCGI Project number: 65

Towards Structural Topology Optimization of Rotating Machinery Considering Fluid-structure Interaction, Turbulence models and 2D-swirl Fluid Flow

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Keywords: Structural Topology Optimization, Fluid-structure interaction, Rotating machinery

Impact: Uncontrolled carbon dioxide (CO2) emissions can have a great influence on the climate
Impact and rotating machineries such as centrifugal compressors and labyrinth seals play and important role in mitigating CO2 emissions. Optimization of these systems might offer designs that are hard to be obtained by intuition or experience. For that, structural topology optimization can lead us to machineries with better efficiency in their operation.

Highlights:
- Topology optimization solutions of stiff structures under fluid-structure interaction and rotation speed.
- Consideration of high Reynolds 2D-swirl flow by using the RANS equations with the k-epsilon and k-omega turbulence models.
- Employment of sequential integer linear programming and CAD/CAE modelling.

Abstract:
This work is associated with the projects "Design of smart labyrinth seals for mitigation of GHG emissions in pneumatic machines" and “Design Optimization of Centrifugal Compressors for Supercritical Gas Mixtures”, from the RCG2I. Design optimization of rotating structural parts, such as in labyrinth seals or compressors, requires the solution of the Navier-Stokes equations that can include complex effects such as swirl flow, turbulence, and fluid-solid equilibrium. While these physics have been employed successfully in the context of parametric and shape optimization, they represent considerable challenges for topology optimization. These challenges include the accurate modelling of fluid-solid walls, imposition of coupling conditions and convergence of the fluid-structure interaction (FSI) equations during optimization. This work employs the method called TOBS-GT that consistently produces well defined and smooth fluid-solid walls, an important to step to add up extra physics or equations in the simulation during optimization. The structural compliance minimization problem subject to volume constraints is solved. The FSI problem is solved via the Finite Element Method considering axisymmetry. Rotational forces are imposed on the structural domain in the radial direction. The 2D swirl flow is governed by the Reynolds-Averaged Navier-Stokes (RANS) equations including a rotating wall in the shaft. The k-epsilon and k-omega turbulence models are employed. Automatic differentiation is employed to compute the required sensitivities. A material model is included in the swirl flow terms to account for the sensitivities of the swirl flow loads on the structure. The optimization problem is solved by using Sequential Integer Linear Programming (SILP). Since solving a 3D-FSI topology optimization problem is computationally costly, the development of 2D swirl flow frameworks is of high interest. Results show that the proposed method can effectively achieve optimized designs of rotating structural parts under FSI loads.

RCGI Project number: 65

Baseline and worn labyrinth seals geometry effect on the leakage evaluation using a numerical approach

Izabel Fernanda Machado; Emilio Carlos Nelli Silva; Shahin Ranjbarzadeh

Keywords: Labyrinth sela; wear; leakage

Impact: This work aims to investigate the wear of labyrinth seals to reduce greenhouse gases

Highlights: The lifespan of labyrinth seals as well as their performance is directly related to the occurrence of wear. There are different types of wear and wear mechanisms, but in labyrinth concisely three types of wear are reported: Rub-groove, plastic deformation, and erosion. A numerical simulation approach of wear in labyrinth seals optimized is presented and discussed.

Abstract:
Compressors and turbines work with pressurized systems at a high rotational speed. Considering aerospace turbines and centrifugal compressors, they work with minimal tolerance for geometric and dimensional deviations to avoid leakage. Labyrinth seals ensure low leakage between different pressure stages in the mechanical systems mentioned above. However, wear is expected. The wear mechanism in labyrinth seals occurs mainly by plastic deformation, rub-groove and erosion. Plastic deformation is characterized by the contact of the labyrinth tooth with the shaft/stator in a process with high strain rates and a high coefficient of friction. Due to the small gap and the repetitive contact between the tooth and the shaft/stator, the tooth of the labyrinth seal forms a mushroom geometry. Abradable materials are used to avoid this plastic deformation of labyrinth teeth. They cushion impacts and protect the teeth. When teeth impact the abraded layers, a rub-groove is formed. Finally, the last wear mechanism in labyrinth seals is characterized by the successive impact of hard particles dragged by the fluid that collide against the surface of the seals, changing their geometry and increasing the wear. This type of phenomenon is known as erosive wear. Therefore, this study aims to develop numerical simulations to predict the leakage of teeth worn by plastic deformation (mushroom) and to quantify the erosive wear in labyrinth seals. The baseline and worn geometries were considered to evaluate the leakage. The proposed wear phenomena will be presented with their formulations in CFD (computational fluid dynamics). The fluid used for the numerical simulations was CO2 to study its reduction in the atmosphere. For the case of plastic deformation, the leakage results will be presented by the difference in the fluid velocity and pressure. While in the case of erosive wear, the erosion results will be presented from the Finnie's model.

RCGI Project number: 65

PERFORMANCE OF POLYNOMIAL EXPANSION IN THE DETERMINATION OF THE 2D VECTOR FIELD OF A BUBBLE FLOW IN AN ELECTROLYZER: AN ANALYSIS BY SYNTHETIC IMAGES

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Júlio Romano Meneghini (USP).

Keywords: Particle Image Velocimetry; Bubble; Electrolyzer

Impact: The images analysis of experiments in electrochemical reactors for the production of hydrogen is essential to solve problems related to both fluid dynamics and the electrolytic process, especially the mixture of oxygen and hydrogen gases.

Highlights: Our new tool determines the field velocities of hydrogen and oxygen gases without interfering with the process, through the addition of tracers or dyes.

Abstract:
The experimental investigation of multiphase flow by image analysis is fundamental in the design, operation and optimization of electrochemical reactors. In the experimental approach, it is possible to record the time-resolved motion of bubbles and/or tracer particles immersed in the liquid to quantify flow parameters (such as TKE, shear stress, vorticity and others) using a CMOS sensor with an LED light source/laser with high acquisition rates. In image processing, the cross-correlation approaches used in PIV (Particle Image Velocimetry) or the individual matching of particle image used in PTV (Particle Tracking Velocimetry) are the most used in the quantification of parameters in the flow in several experiments. However, the addition of tracer particles in the fluid can interfere with the electrochemical process of the reactors, limiting the use of PIV strategies. In addition, the high concentration of H2/O2 limits the individual identification of bubbles, decreasing the performance of PTV analyses. A promising approach may be to use the polynomial expansion (Farneback approach) to estimate the velocity of bubbles/liquid pixel by pixel from a color gradient in a time-shifted image pair. This stage of the work proposes to investigate the performance of polynomial expansion in the investigation of multiphase flow in the electrochemical reactor. The experiment performed by Pang et al. (2020) was used as a basis to analyze the performance of polynomial expansion in estimating the velocity field of H2/O2 bubbles. In this experiment (Figure 2a), the bubble flow in the electrochemical reactor was recorded by a high acquisition rate camera (frames per second) for different Reynolds. In the recording, a LED backlighting system similar to Shadowgraph (also known as shadow PIV) was used to highlight the bubble images. The synthetic image of the bubble generated has an outer diameter (de) range of 10-20 px and the inner diameter was defined as 1\2 of de based on the images from Pang et al. (2020).

RCGI Project number: 56

Protonic conductive electrolytes for high-temperature solid oxide electrochemical cells.

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Keywords: Solid oxide fuel cell; proton conducting electrolyte; perovskites

Impact: Conventional heat engines used worldwide for electrical power generation require biofuels to meet current environmental requirements for pollutant emissions, but their conversion efficiencies do not exceed 20%. Consequently, electrochemical systems, such as SOFC, have become very competitive because of their practical electrical efficiency of more than 60% and the low impact on air pollution.

Highlights:
Intermediate temperature SOFC operation
Proton-conducting electrolytes
Increased mobility and lower proton activation energy
Adequate conductivity at intermediate temperatures
Better SOFC operating conditions
Increased SOFC cell life.
Prepared electrolytes show good stability.
Similar conductivity to commercial materials

Abstract:
Solid oxide fuel cells (SOFC) are promising electric generation systems that are gaining relevance in the energy sector due to their high energy conversion efficiency, low environmental pollution, and potential use of some renewable energy sources such as biofuels. The most developed solid oxide electrolytes used in these systems are oxygen ions conductors that reach adequate conductivities only at high temperatures (above 800°C). In contrast recent proposed proton-conducting electrolytes can get adequate conductivity at intermediate temperatures (400 to 800 °C), resulting in better operating conditions and increased life of structural and active materials.
Currently, the main metal oxides exhibiting protonic conductivity are perovskite structures of the A2+B4+O3 type, in which A2+ are by divalent cations such as Ca2+, Ba2+ and Sr2+, while the B4+ are tetravalent cations such as Zr 4+ and Ce4+.1 Among these two classes, the cerium-based ceramics present higher protonic conductivities at intermediate temperatures (in the range of 400-800°C), although having unsatisfactory chemical stability. On the other hand, zirconium-based materials show good chemical and thermal stability, but their conductivity is not so high at intermediate temperatures. In this work, the synthesis of Ba(0.7)Zr(0.1)Y(0.1)Nd(0.1)Ox material was carried out using a method of co-precipitation of ammonium carbonates followed by heat treatment at 500º C to eliminate carbonates and nitrates. Next, electrolyte pellets were formed with the prepared materials, and these were heat-treated between 1000º-1500º C, and then characterized by X-ray diffraction measurements. In parallel, conductivity tests of pellets formed with a commercial BaCeZrY material treated under Ar and air at 1500oC were carried by impedance spectroscopy. X-ray data indicated the formation of the desired Ba(0.7)Zr(0.1)Y(0.1)Nd(0.1)Ox phase for materials prepared using heat-treatments above 1450

oC; in the case of commercial BaCeZrY, conductivities similar to those reported in the literature have been found.2 In summary, these results evidenced the appropriateness of the materials and pellets preparation procedures employed in this work.

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RCGI Project number: 57

Development of an Electrolytic Concentrator of Vinasse

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Keywords: Sugarcane, vinasse, circular economy

Impact: This project proposes to develop an electrolytic concentrator of vinasse, which generates concentrated vinasse and valuable by-products, namely oxygen and hydrogen, which creates a novel value chain for the agroindustry. This value chain may more than pay off for the novel electrochemical technology and further promotes ways toward negative GHG emissions (i.e. BCCU and/or BCCS), potentially amounting to more than 1% of the annual global GHG emissions.

Highlights:
About 1.7 Billion BRL could be saved by the Electrolytic Concentrator of Vinasse (ECV);
Sugarcane mill could produce green ammonia with a fraction of the green hydrogen produced by the ECV;
Oxyfuel combustion of sugarcane biomass can be habilitated by the ECV and pure CO2 streams would be available for BECCUS;
Sugarcane mills could produce carbon negative commodities;

Abstract:
Agro-industrial processes, such as the production of biofuels, tend to generate large amounts of effluents, such as vinasse, which is a by-product of the sugarcane industry, which has high water content, usually greater than 95%. Vinasse can be used as fertilizer, for example, through fertigation processes, although this is related to economic and environmental constraints.
As a fertilizer, vinasse can represent an economical, low-carbon alternative to commercial synthetic fertilizers, however, when applied to field crops as produced (i.e. in natura), vinasse can cause environmental issues and economic constraints, including, greenhouse gas emissions and high transport logistics costs, respectively.
It is known that the application of vinasse to sugarcane plantations is responsible for promoting a greater release of greenhouse gases, which are related to the burning of fossil fuels (e.g. diesel) by vehicles transporting this wastewater and to promoting greater amounts of greenhouse gas emissions from the soil of sugarcane plantations.
The economic concern is related to the cost of transporting vinasse, which tends to become uneconomical versus synthetic fertilizers, as the distance from the source of production to the point of application becomes considerable. In addition, synthetic fertilizers associate a greater carbon footprint with the commodities traded by the associated agricultural industries.
As described in a recent patent of Prof. Lopes et al., there is no document in the state of the art that deals with the reduction of the volume of agro-industrial effluents, in particular vinasse, through the reduction of the water fraction through electrolysis. Documents were found that deal with the concentration of vinasse by thermal means. Documents dealing with the decomposition of organic matter contained in effluents through electrolysis were also found. Some documents aim to reduce the chemical oxygen demand of vinasse, being in one document, concomitantly, the production of hydrogen for application as an alternative fuel. However, no precedent was found for the use of direct electric current, applied in a direct and controlled manner, for the electrolytic concentration of vinasse. Such a process has as by-products hydrogen and oxygen gases, which can serve as commodities and be used as inputs in oxy-fuel combustion processes, or in the synthesis of synthetic chemical molecules, making the process, as a whole, economically viable and associated with a circular economy concept. Such a value chain was also not found in the state of the art. Both the electrolytic process of concentrating vinasse and this value chain have been included in a patent filed recently by Prof. Lopes et al.

Electrocatalysts for hydrogen production by ethanol electrochemical reforming

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Keywords: 1. Electrochemical reforming 2. Green-hydrogen 3. Ethanol oxidation

Impact: During the last decades, the energy demand has increased with society's development, and predictions pointed out that energy consumption will increase 3-fold by 2050. To be sustainable, alternatives to produce clean fuels as green-hydrogen production from electrochemical reforming of organic molecules such as ethanol and glycerol have been developing efficiently in our group based on MoS2 and PdPt electrocatalysts.

Highlights:

- Non-noble metal electrocatalyst for HER based on MoS2
- The higher stability of MoS2 cathodic material in an alkaline medium
- Ethanol electro-oxidation in alkaline medium with PdPt electrocatalysts
- Ethanol reforming for hydrogen production with a low cell potential of 0.9 V

Abstract:
Hydrogen is the most abundant element in the universe and its importance goes exclusively to industry (chemical and petrochemical) and only a small part goes to its use as an energy matrix (5.68 %), because of the issues around its sources and production. Green hydrogen production from ethanol electrochemical reforming appears as a promising opportunity to increase its participation as future fuel along with ethanol advantages. In this way, electrochemical reforming of small organic molecules, such as ethanol, has been postulated as a promising alternative as a function of refinery coupled processes to obtain clean energy and/or high aggregated value compounds. In addition, ethanol has other promising characteristics like low toxicity, high energy density, high thermodynamic efficiency, and, in Brazil's scenario, a whole fully developed production, storage, and logistics across the country. Ethanol electrochemical reforming is based on ethanol electrooxidation in an anode compartment to form CO2 and 12 H+ ions that migrate to the cathodic compartment to be reduced to molecular hydrogen, and the cell voltage to complete these reactions is around 0.8 V which is lower than hydrogen production from water electrolysis ca. 1.8V. Here this study, there will be described the results to synthesize a fusible and large scalable cathode electrocatalyst based on the electrodeposited MoS2 onto nitrogen-doped carbon support without the dependency of noble metals like Pt. This material presented higher activity in acidic medium (only 150 mV dislocated from Pt/C electrocatalyst), but in alkaline, this material is dislocated only 30 mV from Pt/C. For anodic materials were developed bimetallic PdPt/C in ratios of 4:1, 1:1, and 1:4 of Pd:Pt for application in acidic and alkaline conditions. From the acidic medium, those materials presented regular activity, but for alkaline medium also achieved a better result toward ethanol oxidation. FTIR in situ experiments determined the products as a function of applied potential and identified the CO2 production in potential higher than 0.6 V as HCO3- species because of the pH value, so achieving high efficiency. Therefore, putting together those results obtained individually, as a proof of concept, leads to a cell potential for hydrogen production from ethanol in an acidic medium of 0.8 V and alkaline of 0.9 V operating in a 10 mA cm-2 current density. However, after some time operating in the acid medium, the cell potential needs to increase to 1.0 V, whereas the alkaline system presented only a small increment to 0.96 V to keep the same rate

of hydrogen production during the same period of operation. Is worth pointing out that this activity in alkaline is obtained from the lowest Pt content anodic material besides the higher Pt content necessary for acidic one, characterizing it as a promising material and medium to be applied in commercial reforming devices.

RCGI Project number: 57

Spontaneous conversion of CO2 and sulfite to energy using a photocatalytic fuel cell

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Keywords: Photo fuel cell, semiconductor, solar energy conversion

Impact: Fabrication of a new solar energy conversion device that can capture CO2 and convert it to fuels and electricity in a spontaneous reaction.

Highlights:

- Fabrication of BiVO4/WO3/V2O5 ternary nanostructured oxide photoanodes for optimization of oxidation half-cell reaction.
- Cu2O/CuO photoanodes with an enhanced ability for CO2 photoreduction.
- New photocatalytic fuel cell device equipped with low-cost semiconductor electrodes for greenhouse gas reduction.
- Assembling of a photo fuel cell able to convert CO2 and sulfite ions spontaneously to electricity.

Abstract:
Humanity needs urgently to reduce emissions of greenhouse gases to the atmosphere as well as to develop new and renewable technologies for energy conversion. Photocatalytic fuel cells (PFCs) have been proposed as a pathway to reduce the costs of conventional fuel cells (FCs) by designing new and smart semiconductor materials for harvesting solar energy and concomitantly converting chemical energy directly into electricity with zero carbon emissions. Here, we prepared BiVO4/WO3/V2O5 photoanodes and Cu2O/CuO photocathodes for the simultaneous and direct conversion of CO2, one of the greenhouse gases, and sulfite ions to electricity (without applying bias). The OCV and short-circuit current of the optimized device under one sun illumination conditions are 0.42 V and 0.5 mA/cm2, respectively, with a maximum power output of 0.05 mW/cm2. The photoelectrodes morphology and structural, optical, and electronic properties were extensively characterized to rationalize the operation mechanism of the PFC device. Further optimizations are under research for improving device stability and identifying the liquid and gas products generated at the cathodic and anodic compartments of the cell.

RCGI Project number: 59

Studying Supported Cu & Ag Nanoparticles on 2D MXenes to Enhance C2+ Products at CO2RR

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Keywords: MXenes; CO2RR; C2+ compounds

Impact: GHG (GreenHouse Gases) are certainly one of the most urgent issues that need attention at the moment. CO2 is the most researched due its high concentration at the atmosphere, reaching more than 400 ppm. Electrocatalysis utilizing nanomaterials has proven to be an excellent option for CO2 transformation into valuable chemicals.

Highlights: Electrocatalysis based on 2D MXenes containing Cu & Ag nanoparticles enabled the formation of C2+ products such as C2H2 and CH3CHO, as well as methane and CO. Worth mention that the preparation of the material was made in a eco-friendly green fashion through solvent-free mecanochemistry.

Abstract:
In the last decade, 2D MXenes have been studied due its high conductivity and surface area in addition to the activity and selectivity for CO2 Reduction Reaction (CO2RR) [1,2]. Ag-based catalysts showed high yield of CO from CO2, an important intermediate at the mechanism for making molecules with two or more carbons, also known as more valuable or C2+ products. However, Ag alone is incapable of making C-C coupling. However, since the earliest publications about metals for CO2RR, Cu has demonstrated to be one of the few that can produce considerable amounts of C2+ molecules, for example ethanol [3]. Therefore, materials containing Ag & Cu are showing promising results to enhance the C2+ production, achieving faradaic efficiency (FE) of nearly 40% and 30% with 300 mA cm-2 for ethanol and ethylene, respectively [4]. Meanwhile, there is a need to increase the selectivity for CO2RR compared to the Hydrogen Evolution Reaction (HER), the main competitor reaction. The study of this project is then to combine the properties of Ag, Cu and 2D MXenes to further enhance the FE for C2+ products with good stability and selectivity for CO2RR. Our results on MXene-Cu and MXene-AgCu using Differential Electrochemical Mass Spectroscopy (DEMS) has shown methane, carbon monoxide and ethylene gaseous fragments. Acetaldehyde was also detected by GC-MS for MXene-Cu. These encouraging results indicated that metal nanoparticles supported on MXenes indeed have high potential to transform CO2 into C2+.
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RCGI Project number: 60

Electrochemical CO2 reduction on functional molecule-modified copper surfaces

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Keywords: Electrochemical CO2 reduction, copper catalyst, surface modification

Impact: A new strategy for reducing the hydrogen evolution reaction (HER) and enhancing the selectivity for the electrochemical reduction of CO2 (ECO2RR) to multicarbon products (C2+) using a heterogeneous copper (Cu) catalyst was realized by employing the polybenzimidazole polymer as a surface modifier. The modified Cu electrodes are convenient to prepare and to scale up.

Highlights:
- surface of copper electrodes were modified with the polymer polybenzimidazole
- inhibition of H2 formation by surface modification of copper electrodes
- increasing formation of methane (CH4) and ethylene (C2H4) compared with the unmodified Cu electrode
- extended stability of the copper catalyst

Abstract:
Electrochemical reduction of CO2 (ECO2RR) over copper (Cu) catalysts have demonstrated an unique ability to produce multicarbon hydrocarbons (C2+) and alcohols, such as ethylene and ethanol. However, it remains a significant challenge to design a catalytic system that enables industrial scale conversion of CO2 into C2+ products using electrocatalysts that have selectivity, stability, and high Faradaic efficiency. For example, Cu catalyst is not selective, and 16 different products were identified during ECO2RR. Also, the competing hydrogen evolution reaction (HER) is an important drawback to be overcome in Cu catalysts for ECO2RR. In this regard, one of the strategies is coating of Cu electrodes with organic species. In general, the coating provides an increase in Faradaic efficiencies for C2+ products, a reduction in H2 generation, and an enhancement of the stability of the catalyst compared to the respective electrodes without the coating. These results are mainly associated with the stabilization of intermediates bound to the catalyst surface, the hydrophobicity of the coating layer, and the stabilization of surface Cu atoms due to coordination with the ligands present in the modifier molecule. In addition, the Cu electrode coating process allows for practical scaling up preparation of electrodes for ECO2RR. Herein, we report the use of polybenzimidazole (PBI), a polymer with groups having coordinating sites, and high stability under ECO2RR conditions, for coating Cu bulk electrodes to be use as electrocatalysts for ECO2RR. The modified electrodes are convenient to prepare, involving a two-step synthesis process: i) preparation of the Cu surface by the reaction with nitric acid, and ii) formation of a polymer film on Cu electrode from a PBI solution. The electrochemical mass spectrometry (EC-MS) technique was used to detect the products formed during the electrocatalysis. Our preliminary results showed that the Cu modified with PBI reduced the H2 formation and increased the selectivity to methane (CH4) and ethylene (C2H4) compared to that of the unmodified Cu surface. Also, the modification of the Cu surface with PBI stabilized the active sites for ECO2RR for long periods under operation (total operation >24h) compared to the pristine Cu.

RCGI Project number: 60

Greenhouse gas-based microalgae bioproducts: A potential biotechnology strategy

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Keywords: : phycoremediation, Dictyosphaerium sp., greenhouse gases

Impact: One of the global concerns is the increase of CH4 and CO2 emissions, with negative consequences on global warming. An alternative is to use biotechnology to convert these gases into bioproducts. Microalgae can naturally convert CO2 into O2 through photosynthesis and, under stress, may transform the CO2 into useful compounds for humans, such as carbohydrates that can be fermented to produce bioethanol.

Highlights:

- A strain of Dictyosphaerium sp. isolated from mangrove was able to grow with methane;
- Methane favored carbohydrate production more than carbon dioxide in the strain Dictyosphaerium sp.
- Methane and carbon dioxide can be converted into carbohydrates for later fermentation and bioethanol production

Abstract:

Nowadays, there is a global concern about the increase of greenhouse gas (GHG) emissions, partly attributed to the rapid development of the world economy. In recent decades, the progression of climate change has made the world aware of the requirement to reduce carbon dioxide (CO2) and methane (CH4) emissions and find ways to sequester these gases by reducing their concentration. A potential solution to this unwanted CO2 and CH4 impasse could be seen by exploring approaches to converting these gases into bioproducts such as lipids, pigment, carotenoids, and carbohydrates. The carbohydrates produced by microalgae can be transformed into bioethanol through fermentation, producing third-generation biofuel. Biofuels from microalgae are environmentally friendly, non-toxic, and have strong CO2 sequestration potential because microalgae are photosynthesizing microorganisms capable of fixing 10 times more CO2 than terrestrial plants. Methanotrophic bacteria are able to use CH4 as the sole source of carbon and energy and turn it into CO2 and water. The goal of this study was to isolate a mangrove microalga with the potential to tolerate high CH4 concentrations and to study the effects of CH4 on carbohydrate production. The microalgae identified by molecular biology resulted in 98% of similarity with Dictyosphaerium sp. Three different growth

conditions were tested: headspace with 5% CO_2, headspace with 5% CO_2, and 12% CH_4 (refreshing the atm every 24h) and bubbling 5% CO_2. The results showed that in the cultivation with 5% CO_2 being refreshed every 24h, there was no cellular growth. But, in the cultivation with 12% of CH_4 in the headspace and bubbling 5% of CO_2, the cellular growth was similar, showing that CH_4 was not toxic to the strain. Furthermore, the results of total carbohydrate quantification showed that in the presence of CH_4, 80% of the biomass was composed of carbohydrates, but with CO_2 bubbling, this value was 56%. Further experiments will be performed to understand if methane participates in the production of carbohydrates by the microalgae, i.e., if this strain can consume this carbon. Another hypothesis to be tested is if the presence of methanotrophic bacteria helps the microalgae to grow in the CH_4 atmosphere, living in symbiosis with the microalgae.

RCGI Project number: 61

Restoration of native vegetation for carbon sequestration – Restore.C

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Keywords: Ecosystem restoration; biomass accumulation; ecosystem functioning

Impact: We will present preliminary outcomes on the assessment of opportunities for cost-effective, low-risk carbon sequestration by Cerrado and Atlantic Forest restoration with biodiversity co-benefits

Highlights:
We established 40 hectares of experimental restoration plantations
We installed and managed two flux towers for assessing carbon fluxes in a savanna and a forest undergoing restoration
We established ~600 field plots for carbon stock assessments in different vegetation compartments and reforestation approaches
We created a database of 300,000 hectares of lidar data.

Abstract:
In this presentation we will describe the first activities developed by the project "Restoration of native vegetation for carbon sequestration – RestoreC", which aims to assess the opportunities for cost-effective, low-risk carbon sequestration by Cerrado and Atlantic Forest restoration with biodiversity co-benefits. We developed this first phase of the project through activities in three independent working packages (WP): WP1 (A mechanistic carbon budget perspective in ecosystem restoration), WP2 (biophysical and management determinants of carbon stocking in ecosystem restoration), and WP3 (Remote sensing approaches to monitoring carbon stocks). In WP1, we established nearly 40 hectares of experimental restoration plantations at the Experimental Station of Forest Sciences of Itatinga (Atlantic Forest) and Chapada dos Veadeiros National Park (Cerrado), through which a plant diversity gradient was established and several soil and ecophysiological measurements have been made. Each of these Megasites are equipped with an Eddy covariance flux tower to measure the flows of carbon, water and energy, and data have been collected both in the experiments and in the tower since the beginning of the RestoreC project. In WP2, we established 600 field plots in different restoration areas located across the state of São Paulo, in which we assessed soil, litter, dead wood, and aboveground carbon stocks. In WP3, we integrated the aforementioned field plots with Lidar data, collected through both drones and airplanes), accumulating nearly 300.000 hectares of area. We will present some preliminary results and early achievement. The next phase of the project will be dedicated to the continuation of the activities described in this report, which forms the foundation of the RestoreC project and will allow modelling carbon sequestration and the development of the "The restoration Atlas: A guide for planning C removal by native vegetation in Cerrado and Atlantic Forest" in later stages of the project.

RCGI Project number: 52

Soil carbon sequestration through integrated agricultural systems in Brazil

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Keywords: Nature-based solutions; Agriculture; Soil carbon sequestration

Impact: Based on this broad context, the Ag4C Project is conceptually and operationally structured to measure the potential contributions of different scenarios of IASs (i.e., from more simplified to more diversified integrated agricultural systems) as Nature-Based Solution for increasing C sequestration in Brazil. We believe that is research priority to support land management decision in the adoption of best land-use configurations to achieve the ambitious NDCs assumed by the Brazilian government in the Paris Agreement to mitigate global warming and climate changes. Finally, Ag4C Project also seeks to create social impacts by performing a comprehensive assessment of key ecosystem services that impact human well-being directly.

Highlights: The main objective of this project is to measure the contributions of integrated agricultural systems on carbon (C) sequestration, to help Brazil to fulfil its NDCs in the Paris Agreement.
To achieve our primary goal, the following specific objectives have been established:
i) to measure the soil carbon stock changes induced by the adoption of integrated agricultural systems (e.g., crop rotation system; agroforestry system; crop-livestock system; crop-livestock-forest system);
ii) to understand the mechanisms of storage and stabilisation of C in the soils using fractionation methods and synchrotron-based techniques;
iii) to quantify the soil greenhouse gas (GHG) emissions (CO2, N2O and CH4) in integrated agricultural systems to refine data for national GHG inventories;
iv) to decipher the interaction of soil biota with soil C stabilisation and GHG emissions in integrated agricultural systems;
v) to apply modelling tools for assessing the impacts of land-use change scenarios, and NDC scenarios on C sequestration under integrated agricultural systems in Brazil;
vi) evaluate the impacts of the adoption of integrated agricultural systems on ecosystem service provision in Brazil;
vii) to offer land management and public policy recommendations for supporting effective nature-based solutions to mitigate climate changes and sustainably promote human well-being.

Abstract:
Integrated agricultural systems (IASs) have emerged as sustainable strategies to intensify land productivity by combining annual crop, livestock and/or forestry activities in the same area under different spatio-temporal arrangements. In Brazil, it estimated that 11.5 million hectares had been cultivated with some type of IASs. Among other socioeconomic benefits, IASs have stood out as promising nature-based solutions for enhancing C sequestration and providing essential products to people (e.g., cereals, meat, and wood). Therefore, IAS can be a powerful solution to tackle global food and energy insecurity and climate change in the coming decades. Recognising the potential of IASs to sequester C and mitigate global warming, one of the goals of Brazil's Nationally Determined Contributions (NDCs) assumed in the Paris Agreement is to increase 5 million hectares of IASs by 2030. In that context, the main objective of Ag4C Project is to measure the potential C sequestration of IASs

conducted under contrasting conditions of climate, soil, and management practices in Brazil. To achieve our goals, the project will be organised in four work packages (WPs), which are sequentially logic, inter-linked and complementarity. The WP1 will be focused on technical meetings to provide specific guidelines and monitor the updating of multiple activities of the project. The WP2 aims to review, synthesise and reanalyse available data in the literature related to the main topics of the project (e.g., soil C sequestration, greenhouse gas (GHG) emissions and ecosystem services). It will allow us to review the state-of-art, identify research gaps and create a dataset for parametrising and validating modelling and scenario analysis. In the WP3 we will measure soil C stocks and mechanisms of soil C stabilisation, GHG emissions, C inputs in the soil via above- and belowground biomass of different species (annual crops, grasses and trees), biological interactions with C storage and GHG emissions, and C balances in IASs. These measurements will be performed using multiple methodological approaches and spatio-temporal scales, including intensive field measurements in paired sites (chronosequences) and long-term experiments, and also, specific experiments conducted in the laboratory and greenhouse under controlled conditions. Finally, WP4 aims to apply modern tools for modelling C dynamics and GHG emissions, performing scenario analysis of management and climate changes and assessing ecosystem service trade-offs and synergies associated with the adoption of IASs in Brazil. These activities will be fundamental to integrate data of previous WPs, to scaling up long-term predictions of IAS adoption on C sequestration, evaluate the effectiveness of NDC scenarios to mitigate global warming and investigate the IAS effects on the benefits that humans obtain from the ecosystems (ecosystem services). We expect to identify the best management scenarios of IASs for enhancing C sequestration and other co-benefits, being a valuable scientific basis for helping Brazil to achieve its NDCs in the Paris Agreement. We also seek to create social impact both within the study country of Brazil, as well as in different global contexts where similar NBSs can be applied to mitigate climate changes and promote human well-being.

RCGI Project number: 53

Integrated Agricultural Systems: the solution to the global FEES challenges

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Keywords: Crop-livestock-forestry; sustainable environment; Food and economic benefits

Impact:

- The work will clear doubts about the future of integrated agricultural systems (IAS) as an alternative solution to the global challenges of FEES-food, environmental, and economic sustainability.
- It will serve as a means to highlight the advantages of IAS over other agricultural systems thus, promote the adoption by encouraging the stakeholders in Brazil, and world-wide.

Highlights:

- Many types of integrated agricultural systems (IAS) are practiced in different countries.
- Countries in the tropical and subtropical regions tend to adopt IAS when compared with the temperate regions.
- Brazil ranked top on the list of countries where IAS is either practiced or studied.
- The benefits of IAS are overwhelming with provision of sustainable environment, increase in food production, as well as improved economic returns and livelihood.

Abstract:
A rapidly growing human population has become an issue to mankind because of the increasing demand for food, land, air, water and other resources. Monocultures with inherent intensification approach as specialized farming which is dominant in industrialized and conventional agriculture has caused several negative impacts to the environment, human, and food security due to overuse of chemical inputs (pesticides, herbicides, fertilizers) leading to low food production, increase in weeds and pests, loss of biodiversity, and reduction in soil-related ecosystem services (such as C-stocks and sequestration, nutrients cycling and enrichments, and others). Hence, the necessity for embracing integrated agricultural systems (IAS), a more sustainable agricultural system to address the challenges of farmers at any level. This work aimed at developing an overview of IAS by discussing, and either bringing to memory or filling the gap in knowledge about the globally practiced types of IAS, locations, as well as its potential and possible challenges. For this review work, large volumes of literature on the topic were retrieved from world famous scientific databases by using a search engine. The study observed that there are many types of IAS practiced in different countries with majority found in the tropical and subtropical regions. It was also discovered that some countries such as Brazil and USA ranked top on the list of countries where IAS is either practiced or studied. Further, the work revealed that the benefits of IAS are overwhelming with the provisions of sustainable environment, increase in food production as well as improvement in economic returns and livelihood. It was concluded that IAS is no doubt the 21st Century alternative solution for addressing the global challenges on FEES (food, environmental, and economic sustainability). The work will serve as a means to highlight the benefits of IAS over other agricultural systems thus, promote the adoption by encouraging the stake-holders world-wide.

RCGI Project number: 53

Nature-based solutions: Sustainable development of Latin America

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Keywords: Nature-based solutions; Living soils; Carbon sink

Impact: The presentation intends to contain technical information about nature-based solutions in an easily accessible format and doing so to contribute to SDG 13 (actions against climate change), as well as to SDG 2 (sustainable agriculture), SDG 12 (responsible production), SDG 15 (preservation of life on land), SDG 16 (justice and effective institutions) and SDG 17 (partnerships and means of implementation).

Highlights: If applied in the Americas, sustainable management practices will promote the SDGs and, at the same time, reduce climate change risks. Many are the 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. 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.

Abstract:
Latin America is a region favored by abundant natural resources and diverse cultures. A large portion of it is located between the tropics, where some feasible agriculture and pasture techniques can be much less impactful for the environment than practiced in other parts of the world. Sustainable agriculture and forestry can link to the sustainable use of resources, balanced use of chemical inputs, harmonious relations between human and soil-plants-livestock, and even become a sink to carbon emissions, providing a nature-based solution to climate change. This chapter offers summarised information from primary and secondary sources, which the authors prepared in many papers and reports over the last five years. As such, it consists of established knowledge in the particular field of soil carbon sequestration in agricultural lands and its role in carbon neutrality that represents one of the few strategies available to be applied on large scales and at potentially low cost, therefore combining the benefits to farmers and at the same time, contributing towards the goals set in the Paris Agreement.

RCGI Project number: 53

Computational design of nanomaterials by coupling molecular simulations with topology optimization

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Keywords: nano-engineered structures, topology optimization, optimal properties and design

Impact: The rational design of nanostructures with enhanced mechanical and physical properties is an emerging and largely unexplored field. Materials design at the nanoscale allows tailoring fundamental properties, becoming essential building blocks for advancing existing technologies and developing revolutionary devices with unique properties.

Highlights:

- Coupling between Topology Optimization methods and molecular simulations
- Computational design of nanostructures
- Optimal design with unique properties

Abstract:
The sake of an optimal condition or topology is inherent in us and nature. In metals, atoms tend to be aligned in minimum energy positions to form unit cells, which defines their crystalline structure. Nonetheless, the advance in nanotechnologies has allowed the fabrication of new optimal configurations, enhancing material properties along the process. These achievements are due to the controlling of matter on a scale ranging from 1 to 100 nm, in which the material's morphology, shape, and structure play an essential role in their fundamental properties. The present study combines Topology Optimization (TO) with molecular modelling simulation. TO methods have been widely employed to solve engineering problems, mainly at the macroscopic and microscopic scales. However, at the nanoscale, their usage is still in its infancy. The nanoscale structural optimization is binary by nature, where a design variable should define the existence of an atom (1) or its absence (0). Thus, the Topology Optimization of Binary Structures (TOBS) method emerges as a suitable candidate algorithm. The TOBS method generalizes the binary TO formulation using sequential integer linear programming. In this study, the elastic constants of bulk materials are maximized subject to different constraints at nanoscale. To the best of the authors' knowledge, this is the first study to carry out nanoscale TO employing formal mathematical programming.

RCGI Project number: 68

Topology Optimization for Temperature Swing Adsorption Multi-Staged Fluidized Bed

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Prof. Dr. José Luís de Paiva - USP

Keywords: Optimization, TSA, Fluidized Bed

Impact: Developing tools for TSA systems optimization is beneficial to the Brazilian oil, gas and biofuels industry, as it paves the way for future carbon-negative power generation projects. This research helps to strengthen the national oil and gas industry from a global perspective. In addition to the benefits presented in the system relevant to the subject of the work, the topology optimization formulation may be used as a foundation for optimization formulations for other fluidized bed systems.

Highlights: Topology Optimization Formulation for Fluidized Beds;
Hyperbolic Material Model for Fluidized Beds.

Abstract:
The world economy still depends heavily on fossil fuels as a primary energy source and electricity. As the global community strives to shift toward a carbon-neutral energy matrix, it is necessary to develop technologies that subtract CO2 that has already been emitted (or will be emitted in years to come) and give it an adequate destination by safe storage or conversion into new added-value substances. Within the concept of CCUS (Carbon Capture Utilization and Storage), coined by the IPCC (Intergovernmental Panel of Climate Change), CO2 capture and conversion are the most costly steps because they mostly have not reached technological maturity or face severe technical bottlenecks. Capturing CO2 from flue gases of fossil-fuel-fired power plants, though technically possible, is highly costly due to the large volumes of gas with low CO2 partial pressure (typically 0.05 to 0.15 atm), relatively high temperatures and the presence of trace contaminants (NOx, SOx, among others). Moreover, there is a gap between research with new materials (catalysts and adsorbents), generally on a lab scale, and the design/optimization of the process that will perform the separation and/or reaction on a large scale. The virtual simulation and optimization for the adsorption beds are based on Computer Fluid Dynamics (CFD) and the Topology Optimization method (TOM). The topology optimization method is a generic tool for distributing material within a domain. In the last decades, it has presented significant progress in its implementation and the possibility of exploring existing manufacturing methods. TOM is applied to produce optimized component topology for Temperature Swing Adsorption (TSA) fluidized beds. Improving the TSA components results in an adsorption system capturing more CO2 than the original bed. CFD modelling and topology optimization formulation results suggest that topology optimization may improve the system adsorption capacity by optimizing the internal topology for the system components.

RCGI Project number: 66

Post-combustion CO2 capture from biomass flue-gas through adsorption process

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Keywords: CO2 adsorption. Fluidized bed. Temperature Swing Adsorption TSA.

Impact: The CO2 capture derived from combustion of biomass combines the use of renewable energy and negative carbon emission. This study addresses the future design of adsorption units for capture of CO2 by Temperature swing adsorption (TSA) technology using multiple-stage fluidised beds.

Highlights: Temperature swing adsorption (TSA) using multiple-stage fluidised beds is a promising technology for CO2 capture at ambient pressure.
A mathematical model of a single stage adsorption was formulated. The model was developed using a systems engineering approach, so that it will be easy to extend it to multi-stage configurations and to the desorption process.

Abstract:
The CO2 capture from flue gas derived from combustion of biomass combines the use of renewable energy and negative carbon emission. Temperature swing adsorption (TSA) using multiple-stage fluidised beds is a promising technology for CO2 capture at ambient pressure. The main objective of this study is to obtain criteria and parameters for the design of a large scale continous unit using TSA technology. The most important biomass sources and their processing routes have been identified, with emphasis to the situation in Brazil, so that sugarcane bagasse has been selected and the tipical flue gas compositon from the direct combustion of this biomass. The design of separation of CO2 by adsorption from combustion biomass combustion gases mixtures depends on the knowledge of the adsorbent and the behavior of multicomponent adsorption equilibrium data. The zeolites 13X and 13 XBF were selected as suitable commercial adsorbents and their experimental characterization was performed in terms of textural properties (specific surface area, total pore volume and micropore volume) and 13XBF showed textural properties superior to those of 13X. The adsorption equilibrium experimental data using CO2/N2 (15/85 v/v) mixtures at different temperatures 323, 343 and 363 K were described and validated for both zeolites according to the Sips and Virial extended models. The isosteric heat of adsorption and the selectivity of CO2/N2 were calculated and the selectivity at low pressure (< 2 bar) was greater than 100.

Two models were considered for modeling the continous countercurrent multiple stage gas-solid adsorption system: equilibrium stage model and phenomenological fluidized bed model. The equilibrium stage model is expressed by mass and energy balance and equlibrium equations and assumes gas and solid phases are in thermal and adsorption equilibrium in the stage. The systems os equations was solved by GAMS, so the adsorber capacity was studied as a function of temperature, heat load, number of stages and solid/gas flowrate.
The phenomenological fluidized bed model considers bubble and emulsion phases in gas-solid bed and phenomenological equation for bubble formation, mean velocities and mass and heat transfer mechanisms in these phases. The influence of gas and solid CO2 load, solid/gas flowrate in the adsorber capacity composition is calculated. The comparison of these two models was useful to define the stage efficiency as a function of operational conditions.

RCGI Project number: 66

Turbulent oxy-combustion flame stability diluted with CO2

Helio Henrique Santomo Villanueva e Paulo Henrique dos Santos Santana

Keywords: oxy-combustion. flame stability. combustion regimes.

Impact: Oxy-fuel combustion is a key technology to green energy transition

Highlights:
* Internal recirculation chamber;
* Flame stability;
* Combustion regimes:
** anchored flame;
** lifted flame;
** flameless combustion.

Abstract:
Carbon capture and storage is a set of technologies that reduce carbon dioxide emissions in power plant applications. Oxy-combustion is a promising way for these technologies to reduce CO2. Understanding flame stability changes in oxy-combustion in relation to air-fuel combustion is fundamental for the application of this concept. This work aims to characterize the flame stability of oxymethane diluted with CO2. From the measurement of the emissions of the radical $OH*$, by chemiluminescence, the regimes of anchored flame, lifted and flameless were established.

RCGI Project number: 67

Green hydrogen production in ethanol-fed SOEC systems

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Keywords: Green hydrogen production; Solid oxide electrolytic cell; Cell supported on the electrolyte and cell supported on the anode

Impact: The search for environmentally friendly energy matrices has become vital for the sustainable development of our society. Among several alternatives, hydrogen has attracted 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 the water reduction using biofuels such as ethanol and glycerol.

Highlights: In this work, solid oxide electrolytic cells were developed for green hydrogen production. Two strategies were adopted for cell construction, one starting from a LSGM (Lanthanum gallate, strontium and magnesium doped) substrate and the other starting from a NiO-YSZ (nickel oxide-yttria-stabilized zirconia) substrate.

Abstract:
In this work we developed solid oxide electrolytic cell involving ethanol electrochemical reform for the 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. Processes of constructing two types of cells were developed: in one the cell is built over the NiO-YSZ anode substrate layer (anode supported cell) and the other the cell is built over a LSGM electrolyte layer (electrolyte supported cell).
For assembling anode supported cells, the NiO-YSZ anode composite was first subjected to several heat treatments for incorporation of YSZ and CGO (Cerium Gadolinium Oxide) electrolyte layers. Then, two different cathodic catalytic layers were included; in one case it was composed by LSCF-CGO (Lanthanum strontium cobalt ferrite impregnated with CGO) and in the other the catalyst was NiO impregnated with CGO. For assembling electrolyte supported cells, the LSGM electrolyte was coated with LSMN (Lanthanum strontium manganite doped with Nickel Oxide) mixed with CGO, for constructing both, the cathodic and anodic layers.
Results showed that, when ethanol was used in the anode, the overall performance of the anode supported cell containing the LSCF-CGO cathode was superior to that with NiO-CGO, and slightly inferior to that of a commercial cell. In the case of the electrolyte supported cell, results evidenced a quite reasonable performance of the electrochemical ethanol reforming process. Analyses of the anode and cathode outlet gases streams showed that hydrogen is not only produced in the cathode by water reduction, but also in the anode through the chemical reform of ethanol. Also, the hydrogen gas produced in the cathode contained small amounts of CO, CH4 and other carbon-based compounds. This indicates the existence of crossover of gases from the anode to the cathode, possibly related to the porosity of the electrolyte layer, as confirmed by scanning electron microscopy. In the overall, investigations evidenced promising perspective for application of both types of cells in electrochemical reform reactors, although some optimization of physicochemical properties of components are still required, in particular, the thickness and porosity of the electrolyte layer.

RCGI Project number: 57

CO2 geological storage in Rio Bonito Formation: contribution for negative CO2 emissions through BECCS in southeast Brazil

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Keywords: BECCS, Paraná Sedimentary Basin, onshore Brazil

Impact: In southeastern Brazil, the Paraná Basin is an ideal target for research on the feasibility of CO2 geological storage. Among the rocks in the basin, the sandy sedimentary deposits of the Rio Bonito Formation have long been studied as non-commercial oil and gas reservoirs. The formation contains a wide variety of rock types with different mineralogical compositions, which, a priori, make it a target for CO2 mineral trapping and its safe storage.

Highlights:

- Paraná Basin covers a large area in southern/southeastern Brazil and contains various rock types with potential for CO2 storage.
- The Rio Bonito Formation comprises reservoirs of an oil play and distinct sandstone types with porosity and mineralogical composition, a priori, favorable for CO2 storage.
- Fine-grained sedimentary rocks in the Rio Bonito Formation may be local unconventional reservoirs or seals for CO2.

Abstract:

The history of Paleozoic depositional events that occurred in southeastern Brazil is recorded in the Paraná Basin, which corresponds to an extensive intracratonic depression located mainly in Brazil (1,100,000 km2) and subordinately in eastern Paraguay (100,000 km2), western Uruguay (100,000 km2) and Mesopotamian Argentina (100,000 km2).

The evolutionary history of the basin is polycyclic, enclosing episodes of subsidence and uplift, primarily controlled by tectonic events. Its sedimentary-magmatic package was formed on the paleocontinent Gondwana with a maximum thickness of about 8,000 m. The basin in the Brazilian territory comprises reservoirs with hydrocarbon accumulations, that could be targets for CO2 geological storage due to its confining properties, such as the petroleum system Irati (source-rock), Rio Bonito and Pirambóia (reservoirs) formations, with a shallow depth of less than 3,000 m.

The Rio Bonito Formation corresponds to the fluvial-deltaic-marine deposition installed in the Permian and is divided into three members, from the base to the top: a) Triunfo Mb., basal, containing fluvial-deltaic sandstones, locally associated with coal beds, siltstones, and carbonaceous shales; b) Paraguaçu Mb., intermediate, containing siltstones and gray shales, interspersed with layers of sandstones and carbonate rocks, deposited in a transgressive marine environment; c) Siderópolis Mb., upper, containing layers of sandstone interspersed with beds of clay, carbonaceous shales and coal, originated in a coastal-marine environment, and with predominance of sandstones, siltstones and shales in the São Paulo state. The Rio Bonito Formation is covered by the siltstones of the Palermo Formation, deposited in a shallow marine platform during the Permian, that could act as caprocks for CO2 reservoirs.

The sandy reservoirs of the Rio Bonito Formation have good permo-porous properties (porosity of up to 20%) even at shallow depths (≤ 3000m) and, in some levels, the presence of hydrocarbons may also indicate the occurrence of structural traps and of saline aquifers. Moreover, fine-grained rocks (siltstone, shale and coal) present in the formation may act as CO2 unconventional reservoirs and as an additional seal.

The mineralogical composition of the Rio Bonito Formation includes albite, K-feldspar, calcite, dolomite, zeolite, quartz and clay minerals, some of them of diagenetic origin. Chlorite is the main clay mineral. Highly illitic mixed layers, disordered interstratified illite/smectite, smectite, and corrensite have also been reported. This set of clay minerals could retain CO2 by adsorption.

The obtained results indicate that the Siderópolis Mb. sandstones in the northeast of Paraná state can be targeted for CO2 geological storage, depending on their west-northwest extension and subsurface properties, which have been investigated in this project.

RCGI Project number: 58

Development of materials for hydrogen production via ethanol reform

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Keywords: Hydrogen production; Electrochemical reforming of ethanol; Cathode and anode development

Impact: Hydrogen is considered the fuel of the future, therefore, it is proposed to develop an electrochemical system for the production of clean hydrogen, based on the electrochemical reforming of ethanol at low temperatures, operated by renewable energy sources. It was developed a promising ethanol reforming cell composed by MoS2 and Rh7Pt1/N-CBlack-Pearl, as cathode and anode, respectively, that is able to produce efficiently hydrogen at cell voltage as low as 0.623 V.

Highlights:

- Production of hydrogen by reforming of ethanol.
- High catalytic MoS2 cathode developed for hydrogen evolution reaction.
- High catalytic Pd-Pt and Rh-Pt anodes developed for ethanol electro-oxidation.
- Cell voltage for reforming of ethanol as low as 0.623 V for MoS2/Rh7Pt1/N-CBlack-Pearl system.

Abstract:

Ethanol is an excellent source of hydrogen, specially, in the electrochemical reforming of ethanol, at low temperatures, represented by the following reactions, in acid medium:

Anode reaction: $C_2H_5OH + 3H_2O \rightarrow 2CO_2 + 12H^+ + 12e^-$ (1)

Cathode reaction: $12H^+ + 12e^- \rightarrow 6H_2$ (2)

Overall reaction: $C_2H_5OH + 3H_2O \rightarrow 2CO_2 + 6H_2$ (3)

Reaction (3) represents the reforming of ethanol at low temperatures, 25 °C – 85 °C. This reaction is similar to a steam reforming process (operating at high temperatures: 600 °C – 800 °C). The energetic demanded to produce 1 mole of H2, in a reforming ethanol cell, is of +58 kJ/mol, with a cell voltage of 0.084 V, that it is much smaller than that from water electrolysis (+286 kJ/mole with a cell voltage of 1.23 V), leading to a lower electric consumption. The relatively slow kinetics limitations of reactions (1) leads to cell voltage of 0.7 – 0.9 V, for the ethanol electrolysis cell operating at 1 A cm-2, while for water electrolysis the cell voltage is much higher, of 1.8 – 2.0 V, operating at the same conditions. Thus, the optimization of the electrochemical reforming of ethanol demands the development of efficient, low-cost, and stable catalysts for both, anode and cathode, targeting large-scale and abundant materials must be developed. MoS2 appear as a promising material and it was selected as a candidate for the cathode in electrolysis ethanol reforming cell. MoS2 is a special material because its activity varies depending on how many layers, defects, and edges sites are exposed, which higher edges sites, number of defects and number of layers (1 - 3 layers – almost bi-dimensional material) are factor that increase its activity toward the hydrogen evolution reaction. Thus, incorporation of electrodeposited MoS2 into a high area carbon matrix doped with a nitrogen was used in this study. On the other side, Pd4Pt1/N-CBP, Pd1Pt1/N-CBP and Pd1Pt4/N-CBP, prepared from the method of chemical reduction of metallic precursors in solution containing carbon of high surface area (carbon black pearl, CBP) were used as anode. Another, high catalytic material developed in our laboratories, RhPt/N-CBlack-Pearl, was also employed as anode material. The operational voltage of the reforming cell using MoS2 as cathode and Pd4Pt1/N-CBP as anode, operating at j = 10 mA/cm2, was of 0.961 V, while for, Rh7Pt1/N-CBlack-Pearl the cell voltage was as low as 0,623 V, at the same operational conditions, showing that MoS2 and Rh7Pt1/N-CBlack-Pearl system is a high efficient system for hydrogen generation.

CO2 storage efficiency considering the sandstone units of the Rio Bonito Formation within southwest São Paulo.

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Keywords: Rio Bonito, Hydrocarbon Indications, CO2 Storage

Impact: The current study focuses on presenting the hydrocarbon viability with CO2 storage options within the sandstone of the Rio Bonito Formation. The results will serve as inputs in deciding on the possibilities of engaging supercritical CO2–based enhanced hydrocarbon production events to foster CO2 storage or reservoir exploration dedicated to CO2 storage.

Highlights:

Hydrocarbon viability will foster CO2 storage options within the Rio Bonito Formation, southwest Sao Paulo.

Dedicated reservoir units for CO2 storage are possible.

Newly acquired wireline logs with incorporated 3D-4D seismic data are pertinent to further establish the hydrocarbon viability.

The Rio Bonito Formation has the potential for CO2 storage based on the reservoir's physical qualities.

Abstract:
The study evaluates the CO2 storage efficiency factors peculiar to the Rio Bonito Formation to present the reservoir options and capacity estimation inputs. The wireline logs reveal a predominantly sandstone unit with interlayered shale and sandstone beds within the study location. Petrophysical evaluations indicate hydrocarbon (mostly gas) presence within the sandstone units, which may promote supercritical CO2–based enhanced hydrocarbon production to foster CO2 storage within the field if further studies reveal economically viable reserves. The study shows that the factors that may improve or reduce CO2 storage include depths, potential reservoir thicknesses, reservoir quality and available area usable for CO2 storage. There are thin-bedded layers of sandstones, siltstones and shale, which limits the potential of the affected unit as either reservoirs or seals/overburdens. Reservoirs' physical properties (effective porosity, permeability, flow zones indicator, free fluid index and pre-existing fluids) vary from one point to another, indicating portions with high prospects for hydrocarbon recovery with the CO2 storage. More factors will influence the storage capacity without economically viable hydrocarbon units in the Rio Bonito Formation to enhance production activities. Such factors include reductions in storage areas (Ea), thickness (Eh), and effective flow zone indicator (FZIeff), which is a function of effective porosity (Φeff) and effective permeability (Keff). Suppose further studies reveal viable hydrocarbon wells to encourage production activities; in that case, it will expand CO2 storage possibility, reducing most efficiency parameters' impacts and significantly porosity-related factors. The hybrid reservoir option will foster CO2 storage potential by reducing limitations involving thin-bedded units and storage areas. The results of this study will serve as input in future hydrocarbon exploration activities and the actualisation of CO2 storage within the region.

RCGI Project number: 58

Conversion of CO2 into biopolymers by the regulation of polyhydroxyalkanoates (PHAs) biosynthetic pathway using the photosynthetic cyanobacteria Synechocystis sp.

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Keywords: biopolymers; Synechocystis; polyhydroxyalkanoates

Impact: Carbon sources have been related as a bottleneck for industrial bioplastic production, because of their costs. Thus, the utilization of an inexpensive carbon source feedstock as CO2 represents a potential strategy to increase the contribution of bioplastic to the world plastic market. Through photosynthetic chemical production in cyanobacteria, CO2 will be converted to biopolymers, representing a promising technology for renewable energy, and CO2 and petroleum-dependence mitigations.

Highlights:
- Sequencing of whole genomic DNA of Synechocystis sp. B12, a newer PHA producer cyanobacteria strain
- Identification of PHA-specific enzymes in its genome
- Identification of three strong candidate ORFs for pha genes in B12 strain

Abstract:
Polyhydroxyalkanoate (PHA)-accumulating bacteria will play an essential role in the transition of petrochemical-based polymeric materials to renewable materials. Bioplastics made from biopolymers such as PHA are eco-friendly, biodegradable, and biocompatible. Despite, many bacteria being able to accumulate PHA intracellularly, the production of this class of biopolymers currently does not pay off. The current proposal aims to investigate the upregulation of PHA synthase genes in photosynthetic cyanobacteria mainly from the Synechocystis genus and especially using the recently obtained poly-3-hydroxybutyrate (PHB)-producer strain B12, which was isolated from a mangrove area in Santos, SP, Brazil. In the present study, we sequenced the whole genomic DNA of the newer PHB producer cyanobacteria B12 strain and identified its PHA-specific enzymes. Possible candidate ORFs for phaA, phaB, phaE, and phaC genes were identified by performing a similarity search of the Synechocystis sp. Strain B12 genome with the phaA, phaB, phaE, and phaC sequences of Synechocystis sp. Strain PCC6803. The organization of the pha genes in B12 suggests the presence of three open reading frames (ORFs), composed of phaA and phaB located contiguously and in the same orientation, phaB alone, and phaC and phaE that also are located contiguously and in the same orientation.

RCGI Project number: 61

Unraveling the potential of blue-green algae biomass for bioethanol production

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Keywords: Biofuels, Bioprocess, Biotechnology

Impact: Brazil is the second-largest ethanol producer globally. However, limitations related to using edible sources (1G) and processing lignocellulosic material (2G) enlighten the potential of 3G bioethanol, produced from green and blue-green algae biomass. They do not need arable land or potable water to be cultivated and use only light, CO2, and nutrients for producing fermentable carbohydrates, which can even be obtained from by-products of industrial plants.

Highlights:

- Isolation of an environmental strain of Synechocystis sp. with potential to concurrently produce carbohydrates for fermentation and polyhydroxybutyrate (PHB)
- Approximately 40% (w/w) carbohydrate content obtained with 0.04% CO2 without further optimization
- Up to 2 g/L biomass produced at bench scale

Abstract:

The depletion of fossil fuels, their contribution to the emission of greenhouse gases (GHGs), and climate changes as a consequence of global warming contribute to the search for negative emissions technologies to meet the world's energy demand. As the second-largest ethanol producer globally, Brazil produced 32.6 billion liters of 1G ethanol from sugarcane (first generation) in 2020, contributing to around 27% of the world's production. However, although the feedstock used is renewable, it still is an edible source and requires the use of arable land. For this reason, new alternatives have been sought, such as producing ethanol from sugarcane bagasse, characterized as second generation (2G), and from algae biomass, the third generation (3G). Yet, technological limitations related to processing lignocellulosic material in sugarcane bagasse weaken the production of 2G ethanol. On the other hand, green and blue-green algae biomass is promising as it requires only light, CO2, and low availability of nutrients to produce fermentable carbohydrates. The carbohydrate content in microalgal biomass can vary from glycogen to starch or polysaccharides, molecules that can be fermented in bioethanol by yeasts. Nonetheless, a stressful growth condition is required for carbohydrate accumulation, which leads to reduced cell division resulting in lower biomass yield, thereby questioning the practical feasibility of bioethanol production. For this reason, a two-step strategy is intended to equally target high biomass productivity and enhanced cellular carbohydrate content by optimizing cultivation conditions. Specific conditions that shall be tested comprise nutrient deficiency, light intensity, or increasing CO2 concentrations, to be evaluated according to an experimental design used for optimization studies. The resulting biomass will be submitted to hydrolysis for complex sugars conversion into monomers of glucose to be fermented by industrial strains of Saccharomyces cerevisiae related to the Brazilian ethanol production process. In a future perspective, coupling the production of 3G ethanol to 1G ethanol could be an alternative to maximize its production without the need to expand the planted areas, also contributing to negative CO2 emissions and directing by-products to a more noble purpose. However, the production of 3G ethanol is still a recent and little-explored technology, which lacks technical and scientific development for its production to become economically viable. Within this perspective, the present work proposes a study to increase the carbohydrate content in biomass of photosynthetic microorganisms, which can be fermented for ethanol 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.

RCGI Project number: 61

BIOPROSPECTION AND IDENTIFICATION OF MICROALGAE FROM MANGROVES AS FEEDSTOCK FOR BIOETHANOL PRODUCTION

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Keywords: Microalgae exopolysaccharides biofuels

Impact: The development of urban activities has led to a significant increase in the greenhouse gases (GHG) emissions. In 2018, the GHG emissions as consequence of the energy consumption reached 33.89 billion tons CO2 eq, with an annual increase rate of 2.0%. The production of microalgae biomass through the consumption of CO2 has been highlighted, in recent years, as one of the most effective alternatives to reduce CO2 emissions through its reuse. As photosynthetic microorganisms, microalgae can fix CO2, in the presence of light, water and nutrients, and convert it into organic sources of carbon. In comparison to terrestrial plants, microalgae can be 10-50 times more efficient in fixing atmospheric carbon. The identification of isolated microalgae in this project will enable the search based on the genus biotechnological potential and the best conditions to enhance the industrial interest compounds production and CO2 consumption.

Highlights: -There is a great microalgae biodiversity in Baixada Santista –SP mangroves and a large field to search for potential producers of the different compounds of industrial interest.
- The MIX2 strain culture is promising to be evaluated for exopolysaccharides (EPS) production
- Microalgae exopolysaccharides (EPS) should be evaluated as a source of carbohydrates to be used in different bioprocesses, since it is a carbon souce easy to be extracted.

Abstract:
The production of microalgae biomass through the consumption of CO2 has been highlighted, nowadays, as the one of the most effective alternatives to reduce CO2 emissions. As photosynthetic microorganisms, microalgae can fix CO2 and convert it into different compounds of industrial interest such as lipids for the biodiesel production, carbohydrate for bioethanol and biopolymers for the biodegradable plastics production. More than 35.000 microalgae species are already described resulting in a large field to search for different compounds of industrial interest producers. The present study is a part of the microalgae prospecting project with microalgae strains isolated from mangroves of Baixada Santista–SP aiming to evaluate their biotechnological potential and CO2 fixation capacity. The molecular identification of the microalgae strains will allow the acquisition of information on their cultivation conditions that will enable both to develop efficient bioprocesses as well as the best understanding of the biodiversity associated at mangroves of Baixada Santista, SP. The molecular identification of microalgae, still in progress, was performed through genomic DNA extraction using a methodology based on cell lysis in lithium acetate and 18S rDNA and ITS1-5.8S-ITS2 region sequencing. The partial results showed a great diversity of the strains identified as Micractinium sp. (21.4%), Coelastrella sp. (14.3%), Dictyosphaerium sp. (14.3%), Parachlorella kessleri (14.3%), Chlorella sp. (7.1%), Desmodesmus intermedius (7.1%), Lobochlamys segnis (7.1%), Chlorella sorokiniana (7.1%) and Chlamydomonas sp. (7.1%). These genus have been reported by our research group to have ability to grow in CO2 atmosphere accumulating lipids and carbohydrates for biofuels production. Regarding the strains not yet identified, the highly viscous MIX2 culture showed to be promising for the exopolysaccharides (EPS) production. EPS, being extracellular, can be considered as a carbohydrate source easily to be extracted by ethanol precipitation. Also, studies related to biofuels production from

exopolysaccharides as carbon source have not been found. In this period, the EPS extraction methods were standardized as well as the analytical methods for the experiment in progress aiming to obtain the microalgae growth and EPS production kinetics and its percentage of carbohydrates. An important aspect is that the production of carbohydrates, lipids and EPS is favored under stress conditions of microalgae cultivation. In this way, the viscosity of the MIX2 culture, as consequence of the EPS production, is explained by the fact that microalgae are possibly isolated in locations that favor the cellular stress condition, since the mangrove in the State of São Paulo is considered a degraded area due to intense occupation, urbanization and industrial pollution.

RCGI Project number: 61

A new protocol for the synthesis of carbamates and isocyanates from CO2

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Keywords: carbamates, isocyanates, polyurethanes

Impact: Isocyanates are currently employed in the worldwide industry of polyurethanes, paintings, coatings, elastomers, adhesives, and sealants. Generally, they are prepared from toxic phosgene. Replacing phosgene from other key and sustainable chemicals, such as CO2 would turn the use of isocyanate much more attractive. The same is true for carbamates, one of the main protecting groups for nitrogen compounds, which are prepared from chloroformates that are also derived from phosgene.

Highlights: A new method to prepare several carbamates and isocyanates from CO2 is disclosed.

Abstract:
Carbon dioxide has proven to be an important source of a one-carbon building block in organic synthesis since it is a renewable raw material, economical, abundant, and with low toxicity. Physiochemically, CO2 is a thermodynamic and kinetic stable molecule, however, it can be transformed into value-added compounds using a suitable chemical environment. In addition, carbamates are important amine-protecting groups and platforms in the synthesis of isocyanates. Isocyanates, in turn, are the main monomers to prepare polyurethanes, but are generally prepared from toxic phosgene. The work presented herein showcases the synthesis of carbamates and isocyanates from CO2 and amines using mild reaction conditions, employing DBU or supported PS-DBU as catalysts. We evaluated different solvents, reaction times, and catalytic systems (homogeneous and heterogeneous) for the capture and subsequent transformation of CO2 into carbamates and isocyanates. We found that in a one-pot procedure the carbamic acid intermediate, formed between DBU, CO2 and amine, can be transformed into carbamates using alkyl halides as the alkylating agents or into isocyanates using POCl3 as a dehydrating agent. The procedure is simple and isolated yields are obtained up to 95% at room temperature.

RCGI Project number: 62

Greenhouse gas emissions in crop-livestock and crop-livestock-forestry systems in Brazil: a bibliometric analysis

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Keywords: Science Mapping, Low-Carbon Agriculture, Greenhouse Gases

Impact: In the scenario of global warming and climate urgency, science must develop and alert for greenhouse gas (GHG) mitigation alternatives. We revealed the leading institutions, authors, and network collaborations on published Brazilian GHG field assessments in diversified-integrated farming systems. We believe these systems are crucial for capturing and storing carbon, mitigating agriculture GHG emissions, and enhancing sustainable productivity.

Highlights:
A bibliometric analysis of GHG field assessment literature in integrated farming systems was performed.
We retrieved 202 papers published from 1990 to 2022 with 27 citations per document.
USP, UFRGS, EMBRAPA, UNB, and UFPR were the top five institutions with more publications containing the most relevant authors.
Brazilian society must join efforts to these existent major players' experience to obtain consistent actions to mitigate GHG agriculture emissions.

Abstract:
Global warming is increasing along with greenhouse gas (GHG) emissions. Brazilian agriculture contributes about 27% of the CO2e emitted in Brazil. Productive systems that integrate agriculture, livestock, and/or forestry are fundamental tools to mitigate these emissions. However, estimates of their potential contribution to reducing GHG emissions and fixing carbon are still imprecise, and the published research remains unintegrated. This study is the first step to refining the literature data and improving net GHG estimation for these agricultural systems in Brazil. We carried out a bibliometric analysis after a systematic literature mapping. Three databases (Scopus, Web of Science, and Dimensions) were used throughout a long-structured line of searching terms for recovering published articles, encompassing the following thematic: (i) greenhouse gases; AND (ii) Brazilian territory; AND (iii) pastures or agriculture as a reference; AND (iv) integrated farming systems as a research focus; AND (v) exclusion of bioenergy, remote sensing or specific modeling approaches. Scopus, Web of Science, and Dimensions retrieved 564, 688, and 577 documents, respectively. The three databases were merged, eliminating duplicates using the bibliometrix package in R v.4.1.2, resulting in 980 different papers. By reading the abstract section, we eliminated studies that persisted: (i) not carried out in Brazil; (ii) not assessing GHG or agricultural areas; (iii) using only modeling without field measurements; and (iv) under laboratory-controlled conditions. After this, 202 documents remained, published between 1990 and 2022, yearly increasing publications by 8% on average, with a high citation per document (27.39). There was a high frequency of the terms "nitrous oxide", "methane", and "carbon dioxide", and a low frequency of "crop-livestock" and "integrated systems", indications that the review is heading in the right direction, but many articles will be eliminated in further full document reading because probably several still don't evaluate integrated systems. Researchers from USP (e.g., Cerri CC; Piccolo MC; Cerri CEP), UFRGS (e.g., Bayer C; Carvalho PCF), and EMBRAPA (e.g., Alves BJR) stood out in collaboration networks. Collaborations involved the Americas, mainly Brazil and the United States, Europe, and Australia. Our science mapping revealed crucial players in GHG field assessments in low-carbon agriculture. Research institutions and scientists' national and international collaboration networks were identified as the current growth of scientific literature on the thematic. The scientific

community, the public policy developers, and society must join the efforts with these major players, learn about their experience, and obtain consistent actions on integrated farming systems to help Brazil achieve the mitigation goals presented through the NDC in the Paris Agreement.

RCGI Project number: 53

Nature-based solutions for climate change mitigation: a literature overview

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Keywords: scientometrics, climate mitigation, soil organic matter

Impact:

Highlights:

Abstract:
As climate change mitigation initiatives develop, new approaches are created to address specific subjects or strategies. Nature-based solutions (NbS) is an emerging initiative centered around working with nature and harnessing biodiversity to protect ecosystems and uphold human wellbeing. We conducted a bibliometric analysis to uncover the main research topics, as well as the main countries involved in developing this new strategy. The string query used in the Scopus database (title, abstract, and keywords) was "nature-based solution*" OR "natural climate solution*", restricted to peer-reviewed papers. We then tabulated the number of papers per country of affiliation for quantitative analysis. We also assessed keyword co-occurrence with the VOSViewer software, restricted the map to keywords with at least 25 occurrences, and removed country names from the keywords list. Of the 1,898 documents retrieved, almost 83% were published in the last three years (2020-2022). The main research subjects involved in the publication are environmental science, social science, and agricultural and biological sciences. Of the 20 countries with the most publications, 15 were European developed countries, with only China and Brazil as emerging countries. Keyword network analysis showed four clusters: i) nature-based solutions and ecosystem services; ii) climate change mitigation; iii) risk reduction and resilience; iv) degradation and pollution. Overlay function revealed a shift from urban-focused research to biomass production and carbon sequestration in soils, suggesting a new trend in research centered around agriculture and forestry solutions. Therefore, for the NbS initiative to effectively reach its goals, the involvement of emerging countries with developed agricultural and forestry industries should be further encouraged, emphasizing the importance of ecosystem management that promotes soil C sequestration as a means for climate change mitigation.

RCGI Project number: 53

Improving pasture management as NBS for soil carbon sequestration in Brazil

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Keywords: Nature-Based Solutions; Pasture; Soil carbon stock

Impact: Management practices are crucial for determining the success of Brazil's NDC alongside with pasture management systems. Besides being critical to Brazil achieve its NDC commitments, such effort would be a useful tool for the evaluation of ABC Program (Brazil´s Federal Program that deals with the organization and planning of the actions to be carried out for the adoption of sustainable production technologies, selected with the objective of responding to the country's greenhouse gas emission reduction commitments in the agricultural sector.

Highlights: The main objective of this project is to evaluate the contribution of improving pasture management systems as a nature-based solution for enhancing soil carbon sequestration in Brazil. This objective is in accordance with the Nature-Based Solution Program's goal (as a part of the RCGI new phase) which is to promote the development of sustainable solutions that help Brazil to fulfil its goals in the Paris Agreement aiming to mitigate global warming, as well as to support the provision of ecosystem services, encourage social well-being and support the elaboration of public policies.

Abstract:
Based on the relevance of improving pasture management systems for soil carbon sequestration and consequently climate change mitigation, some of the commitments of the Brazilian government in the Nationally Determined Contribution (NDC) are related to the restoration of additional 15 million ha of degraded pastures. However, the effects of pasture recovering in soil carbon stock changes and its relevance for Brazil achieve the NDC commitments remains largely unknown. In this sense, this project aims to evaluate the contribution of improving pasture management systems as a nature-based solution for enhancing soil carbon sequestration in Brazil. To do so, project activities are organized into four work packages, as illustrated in Figure 2. The first work package is dedicated to the synthesis of available data. The central part of the project (work package III) is related to measurements of soil carbon stocks, greenhouse gas emissions and assessment of soil microbiology. In work package IV, we will perform a data integration using modelling and scenario analyzes. Thus, apart from considering the provision of ecosystem services other than the agricultural production itself and carbon storage, one should also consider that pasture systems are also subject to climatic extremes and climate change and will need investments for adaptation, which may affect their implementation at a given place.

RCGI Project number: 54

Estoque de carbono orgânico do solo (C) em fitofisionomias campestres ou de savana não antropizadas nos biomas do Brasil, uma revisão sistemática de dados publicados

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Keywords: Campos, savana, estoque de carbono

Impact: Estudos sob as fitofisionomias campestres ou de savana no Brasil, envolvem atributos relacionados com o clima, a vegetação e o solo. Compilamos informações publicadas nos últimos 30 anos sob estoques carbono orgânico do solo nas fitofisionomias campestres e de savana não antropizadas. Isto constitui um ponto de referência para entender os impactos que os manejos (antrópicos) da agricultura ou da pecuária exercem sob os estoques de carbono do solo nestas fitofisonomías

Highlights:

Recopilou-se informação de 137 documentos (artigos científicos, tese e dissertações) contendo informação de C na camada 0 - 30 cm e 64 documentos na camada 0 – 100 cm.

Recopilou-se dados de C de 496 perfis de solo amostrados na camada 0 – 30 cm, e 215 perfis na camada 0 – 100 cm.

Elaborou-se uma base de dados de clima, atributos do solo e C das fitofisionomias Caatinga, Campos de altitude do sul do Brasil, Campos de altitude do sudeste, Campos do Pampa, Campos do segundo planalto, Campos rupestres e Savana.

Abstract:
Os ecossistemas campestres e de savana do Brasil são fornecedores de diversos serviços ecossistêmicos, dentre eles o potencial de armazenamento de carbono orgânico (C) no solo. No contexto atual de discussão sobre adaptação às mudanças climáticas, se faz necessário consolidar dados e informações sobre os estoques de C em diferentes profundidades do solo em fitofisionomias campestres e de savana não antropizadas. Isto permite gerar valores de estoques de C que possam ser utilizados como referencias ou pontos de partida, quando se avaliem os efeitos da melhoria dos sistemas de manejo de pastagens no sequestro de carbono do solo no Brasil. Permitirá testar cenários alternativos de manejo das pastagens como previsto no projeto RCGGI A.3 Improving pasture management as NBS for soil carbon sequestration in Brazil, pelo que ter conhecimento detalhado do status quo do C das savanas não antropizadas se torna de grande interesse.
Uma revisão sistemática de literatura disponível em meio digital foi realizada, com o objetivo de obter dados originais de C (%), densidade do solo (DS Mg m-3) e estoques que C (Mg ha-1), do solo em ecossistemas campestres. Foram consultados artigos teses e dissertações publicados desde o ano de 1990 nas bases de dados Web of Science, Science Direct e na Biblioteca Digital Brasileira de Teses e Dissertações. Foram obtidos dados de C das camadas mais superficiais até 100 cm de profundidade, o bioma, fisionomia da vegetação, classe de solo, textura, coordenadas geográficas, região e município. As buscas foram delimitadas, utilizando termos para as pastagens naturais como: campo nativo, grassland, grassy, savana, savanna, native pasture, rangeland; para os biomas foram utilizados os termos Pampa, campos sulinos e cerrado. Uma base de dados foi construída, contendo informações de atributos do solo e estoques de C das fitofisionomias campestres e de savana. As informações coletadas

de carbono orgânico do solo nos perfis amostrados até a camada 0 - 100 cm, revelam como valor médio de estoque de C: 394 (±10), 139 (±47), 225 (±69), 203 (±8), 115 (±72) Mg ha-1 nas fitofisionomias Campos de altitude do sul do Brasil, Campos do Pampa, Campos do segundo planalto, Campos rupestres e Savana, respectivamente.

RCGI Project number: 54

Impact of competitive adsorption of H2O and SO2 on CO2 capture by 13X zeolite

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Keywords: CO2 adsorption, 13X zeolite, water vapor, SO2

Impact: Biomass combustion combined with CO2 capture from the flue gases is considered a renewable energy source with low carbon footprint. This study addresses the impact of contaminants (H2O, SO2) ordinarily present in flue gases on the capture performance of zeolite 13X, a benchmark CO2 adsorbent.

Highlights: The uptake of CO2 by zeolite 13X is significantly affected by the presence of water vapor, even at low relative humidities. The adsorption isotherm of CO2 may be adjusted to account for partial pressure of water. The exposure of the adsorbent to SO2 drastically decreases CO2 uptake because of irreversible reactions with the zeolite structure, which significantly reduce available micropore volume.

Abstract:
This work aims at studying the effects of the presence of H2O and SO2 in flue gas streams on the performance of CO2-adsorbents. Commercial Binder Free zeolite 13X (13XBF) was considered as a benchmark adsorbent and adsorption equilibrium and kinetic data were measured on a magnetic suspension balance (MSB) for pure CO2 and after exposure to either water vapor or SO2 in a pre-adsorption step. It was observed that 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 after SO2 adsorption, i.e. the reduction of about 35% of the total pore volume. Contact times of up to 3 hours between 13XBF and SO2 diluted in helium (4500 ppm) allow for the recovery of the starting material, which was not possible after contact time of 12 hours neither at 50 °C nor at 70 °C. Regarding water vapor pre-adsorption, the higher relative humidity the adsorbent is exposed to, the largest is the drop in CO2 uptake. Nevertheless, unlike SO2 adsorption, the adsorption of water vapor is reversible if the adsorbent is heated up to sufficiently high temperatures (typically 300ºC).

RCGI Project number: 66

Numerical structural analyses of centrifugal compressors operating with co2 in a supercritical state

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Keywords: structural analysis, fluid-structure interaction, optimization

Impact: The most frequent failures of centrifugal compressors are directly related to fatigue. This can occur due to imbalance, operation under unstable conditions, or in resonance region that generates excessive vibration. The work, then, grouped in a single optimization framework the static and dynamic structural disciplines. Making possible the design faster and structures with longer service life.

Highlights: A computational framework capable of integrating both static and modal analyses was developed for use in the design of centrifugal compressors. Resonance identification methods based on Campbell Diagram were implemented and employed as objective functions in the optimization. A static stress analysis methodology was developed, as well as a set of design requirements for a centrifugal compressor.

Abstract:
Carbon dioxide (CO2) is the main greenhouse gas (GHG), and its presence in the atmosphere has increased from 280 ppm in 1750 to more than 400 ppm in the current years. Therefore, in addition to the direct reduction using new sources of energy, it is necessary to advance toward Carbon Capture, Storage, and Utilization (CCSU) technologies. The research focused on CCSU is expanding knowledge on the use of CO2 in a supercritical state (sCO2). The use of sCO2 as a working fluid enables more compact and efficient equipment in both transportation and power generation cycles. However, their properties have a highly nonlinear behavior near the critical point. But the use of inlet conditions close to this region maximizes the advantages of sCO2, corroborating for new research to be carried out to improve the numerical design models. Regarding the structure, the use of sCO2 as a working fluid provides the construction of more compact structures, reducing the mass of the components as well as the cost of materials. Nevertheless, due to the high specific mass, the aerodynamic loads resulting from the fluid-structure interaction have a larger amplitude. This directly affects the impeller's vibration frequencies, modes shape, and static behavior. Therefore, careful studies of the structural failure modes and modal analysis to verify resonance are essential to ensure structural integrity and to design components with long service life.

RCGI Project number: 77

Design Strategy for Enhanced Oil Recovery Compression Systems Operating with S-CO2

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Keywords: Carbon Capture, Utilization and Storage; S-CO2 Centrifugal Compressor; Gas-like Behavior Margin

Impact: The design strategy developed for Enhanced Oil Recovery compression systems using 1D and CFD models of centrifugal compressors, reduced the total power in 14.09% and avoided high thermodynamic properties variation that could jeopardize CFD model convergence. Moreover, the high-dimensional CFD model optimization improved fluid flow in the machine.

Highlights:
- Total power of EOR compression system reduced by 14.09%;
- Gas-like Behavior Margin is proposed;
- 'Entropy-guided' phenomenology analysis for S-CO2 centrifugal compressor.

Abstract:
The rising importance of carbon capture, utilization and storage (CCUS) industry due to global warming has increased the development of new technologies. Centrifugal compressor train is an essential system required for the storage of supercritical CO2 into oil wells, a process known as Enhanced Oil Recovery (EOR). The compression system design approach used in this work is composed of an optimization methodology based on one-dimensional (1D) centrifugal compressor model, capable to predict the fluid flow aspects that are not modeled through direct thermodynamic analysis, followed by a Sensitivity Analysis (Morris and SS-ANOVA) and response surface (RS) optimization strategy for large and high-dimensional computational fluid dynamics (CFD) models of supercritical-CO2 centrifugal compressor impeller and vaneless-diffuser. Furthermore, a Gas-like Behavior Margin (GBM) is presented to avoid high variations of thermodynamic properties on the compression process close to the widom-line which can difficult the numerical convergence for the CFD approach and also can cause damage to the equipment. The optimal centrifugal compressor train with four stages reduced the total power consumed by 14.09% when compared to the baseline configuration, ensuring that the fluid flow constraints as the Acceleration Margin to Condensation (AMC), GBM and Mach number at the throat are met. Moreover, a CFD modeling for the fourth stage of compression was built which demonstrated good agreement with 1D modeling and experimental data, proving the validity of using the methodology developed herein, as a fast and low-cost way to obtain a high-performance design of centrifugal compressors train system. Finally, the s-CO2 centrifugal compressor CFD model optimization further increased its polytropic efficiency in 1.19%, diminishing total entropy generation in 8.5%. From phenomenology analysis of the dynamic flow was identified that the narrowing of the vaneless diffuser has extinguished the recirculation present in the original geometry's impeller/diffuser interface region and that the enlargement of the impeller's meridional profile has smoothed the fluid flow change of direction (from axial to radial), displacing the swirl structures that restricted the fluid flow in the main passage. The strategy adopted herein can be applied to high-dimensional CFD models to reduce the computational cost with suitable results regarding fluid flow phenomena.

RCGI Project number: 77

Topology optimization of compressible flows using TOBS-GT method

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Keywords: Compressible Subsonic Flows, Topology Optimization, TOBS-GT

Impact: This work proposes to expand the implementation of the TOBS-GT method to compressible flow problems paving the way for future applications in more complex flows, such as turbulent supersonic flows. Also, it is important to have different kinds of TO approaches, for the cases where one can not handle the problem, another can be used. Moreover, there are more types of boundary conditions in compressible flows than in incompressible flows. Depending on the characteristics of the simulations, a determined set of boundary conditions can be more suitable than another. In this work, the Dirichlet boundary conditions of static temperature and static pressure were used at inlets in place of velocity and enthalpy profiles used in the literature. The modifications in the boundary conditions and TO methodology change the behavior of the entropy-based objective function sensitivity, often used in compressible TO problems, in such a way that is necessary to propose a new objective function (i.e., maximization of mass flow rate) to ensure that the optimizer does not converge to a trivial solution.

Highlights: The application of topology optimization to compressible flow problems without porous solid and with a clear interface between solid and liquid.

The utilization of a new set of boundary conditions at inlets in the topology optimization of compressible flows.

An alternative objective function to minimize entropy in compressible flows which avoids the trivial solution of zero velocity field.

Abstract:
Incompressible fluid flow includes a vast quantity of optimization engineering problems. However, depending on the flow characteristics, the compressibility of the fluid is no longer negligible, and the flow becomes compressible. Currently, the fields of energy generation and gas leakage control (where the flows are intrinsic compressible) have been receiving special attention in order to mitigate the greenhouse gases emissions and, consequently, climate change. To the best of the authors' knowledge, the work of Sá et al. (2020) was the first to apply the topology optimization (TO) in laminar and compressible flows using density-based approach. Density-based models have been successfully applied to many fluid flow problems over the years. Nonetheless, the approach presents some well-known drawbacks, such as: the optimization parameters have a high impact on the result being often determined by a cumbersome trial and error process, the presence of elements with intermediate pseudo-densities values, which may lead to artificial physics simulation, and spurious pressure gradient inside the solid regions. Recently, an alternative approach called Topology Optimization of Binary Structures with Geometry Trimming (TOBS-GT) was proposed by Picelli et al. (2022), aiming to reduce the influence of the optimization parameters and eliminating the presence of pseudo solids. The TOBS-

GT method consistently produces a clear interface between fluid and solid by trimming the solid regions from the design domain. This work expands the application of the TOBS-GT method to subsonic compressible flow problems under a low Reynolds regime. It was found that mass flow maximization was able to, indirectly, minimizes the entropy generation. Two cases are evaluated, a traditional double-pipe and bend-pipe.

RCGI Project number: 77

The role of water for the CO2 uptake in clays

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Keywords: Carbon capture, clay, molecular modelling

Impact: Clays are materials with the potential for carbon dioxide storage due to their swelling capacity. However, there are some specific conditions to enhance this process. Our work discusses the important role of water in the CO2 uptake in the fluorhectorite smectite. These findings can lead to process optimization for CO2 storage in the subsurface.

Highlights: The work combines experimental and simulation approaches where both complement each other for a better understanding of CO2 uptake in clays. The authors observed the CO2 entrance in the clay interlayer space will not occur in the case of dehydrated clays, showing that water plays a central role in the clay swelling resulting from the CO2 injection.

Abstract:
A more sustainable alternative for carbon capture and storage can be clay minerals, particularly expandable clays like smectites. Clay minerals are interesting in the context of carbon storage as they are low cost, naturally abundant in Brazil, and can adsorb considerable amounts of CO2. Due to their relevance in soils and several uses as building materials, dye remediation, medicine delivery systems, or built barriers in the management of radioactive waste, the water in clay minerals plays a specific role in several processes. Understanding these materials at the molecular level will help you manage and monitor their swelling behaviour for these applications. In our work, both experimental and simulation approaches were combined to better understand the intercalation mechanisms of CO2 in dehydrated and hydrated synthetic Na-fluorohectorite clay. The employed methodologies were powder X-ray diffraction, inelastic and quasi-elastic neutron scattering, and density functional theory calculations. The studies emphasize how CO2 and water interact at the molecular level in the 2D interlayer of synthetic hectorite. We observed that just for the hydrated Na-fluorohectorite we may obtain crystalline swelling or spectroscopic changes in response to CO2. From the simulations, we conclude that intercalated water molecules decrease the layer-layer cohesion energy and create physical space for CO2 intercalation.
We can now show that, relative to bulk aqueous water, interlayer confinement lowers the Na+ hydration number, which may facilitate proton transfer, hydroxide production, and CO2 adsorption as carbonates. These findings can lead to process optimization for CO2 storage in the Brazilian context. In addition, this study can be expanded to other relevant minerals for carbon storage.

RCGI Project number: 58

CO2 geological storage in Rio Bonito Formation coalbeds integrating a BECCS system

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Keywords: CO2 adsorption, unconventional reservoirs, Paraná Basin..

Impact: Coalbeds are efficient and safe reservoirs to CO2 geological storage, due to its sorptive storage capacity and the associated CO2 adsorption trapping mechanism. The CO2 storage capacity of coal is so significant that coalbeds of Rio Bonito Formation can be targeted for CO2 geological storage of approximately 5.4 Gt of CO2, integrating a BECCS system, where coal act as both a reservoir and caprock to the CO2 captured from ethanol producing units in São Paulo State.

Highlights:

- Coal can act as a CO2 source but also as a CO2 sink.
- Coalbeds have dual properties and act as unconventional reservoirs and caprocks.
- Rio Bonito Formation coalbeds have ideal organic and mineralogical components for CO2 geological storage despite the high level of heterogeneity.
- The coalbeds of Rio Bonito Formation are interbedded with sandstones, configuring a hybrid (multi-lithology) type of reservoir, with additional storage capacity due to CO2 adsorption.

Abstract:

Facing the potential for bioenergy coupled with carbon capture and storage technologies (i.e., BECCS) in the southeast region of Brazil, this study presents the geological storage capacity assessment within this region, to support net-zero goals and to provide negative CO2 emissions by permanently storing significant amounts of CO2 in the subsurface. The objective is to identity and characterize potential reservoirs to CO2 geological storage, as well as determine the CO2 storage capacity and caprock integrity of the system.

The potential for BECCS in SE Brazil comes from synergies between carbon dioxide source and sink: there is a high concentration of bioethanol production units that lay on top of the largest South American sedimentary basin, the Paraná Basin, which present geological favourability to CO2 storage. Such favourability its attributed to the occurrence of hydrocarbon accumulations, saline aquifers, and of coalbeds, attributed to the Rio Bonito Formation, which are favourable lithologies to CO2 trapping that contain the required reservoir properties and confinement (Bachu et al., 2002; 2007).

Worldwide, coalbeds are important reservoirs to CO2 due to its sorptive storage capacity and the competitive adsorption between CH4 and CO2. Additionally, due to the CO2 adsorption trapping mechanism, coalbeds could be effective shallow CO2 reservoirs (no need to ≥800m depth).

This study is inserted in this research context and focus on the role Rio Bonito Formation coalbeds as CO2 reservoirs. The main objective is to determine if coalbeds are feasible targets for CO2 geological storage in the Paraná Basin, or if these would behave as permeability barriers to CO2 storage and act as caprocks. The hypothesis is that both situations occur and depend on the local geology. This is due to the high level of heterogeneity of coal and of the Paraná Basin geological formations in general, attributed to major events of magmatism and associated igenous intrusions along the basin. The research methodological framework comprises a general characterization of the Rio Bonito Formation coalbeds, followed by a detailed analysis of the organic and mineralogical content of studied samples. Additionally, gas sorption isotherms measurements and reservoir properties will be addressed to estimate the porosity, permeability and CO2 storage capacity of the coalbeds. The methodological framework is in accordance with previous research. (e.g., Bachu et a., 2007; Busch & Gensterblum, 2011).

Obtained results indicate that coalbeds in Rio Bonito Formation (Bonito and Barro Branco coal layers) have ideal organic and mineralogical components for CO2 geological storage. However, due to the high level of heterogeneity (due the thermal influence of igneous intrusions – characteristic of the Paraná Basin), storage capacity estimates should be local.

RCGI Project number: 58

Multiscale modelling of reactive transport and CO2 mineral trapping mechanisms at the Rio Bonito geological formation

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Keywords: Atomistic simulations, CO2 mineralization, geochemical trapping.

Impact: This work aims to provide a complete multi-scale molecular description of the Rio Bonito formation, located in the Paraná Basin, to build accurate reservoir-scale models for the CO2 mineralization process. The multiscale molecular simulations will help to evaluate important physicochemical properties of the fluid-rock interface, CO2 diffusivity, steps of mineralization reactions and phase changes of the geological components of the formation.

Highlights:
- Equilibrium properties and transport coefficients of the aqueous phase (density, viscosity, diffusivity, solubilities, etc.);
- Fluid-rock interfacial tensions;
- Reaction rates associated with chemical processes at the mineral substrate;
- The reservoir's permeability curves – with all of these parameters evaluated at the range of thermodynamic conditions found at the geological site.

Abstract:
The growing concern with the climate changes caused by the emission of greenhouse gasses (CHG) in the atmosphere, among them carbon dioxide CO2, has led to the search for technologies capable of mitigating the impact caused by these pollutants. One of the alternatives that have shown promise is the capture and storage via geochemical trapping, through the mineralization process. Molecular dynamics and reactive transport simulations will be used to investigate the CO2 mineralization process following its injection in a Brazilian geological formation, more precisely, the Rio Bonito formation in the Paraná basin. The mineralization problem requires a multi-scale modelling approach, starting from a molecular-level assessment of fluid-rock interface properties, including surface chemical reactions, followed by a characterization of the rock's porosity profile and, finally, the consistent incorporation of this data into a reservoir-scale flow model. In this context, our research project plan targets the determination of (a) equilibrium properties and transport coefficients of the aqueous phases (density, viscosity, diffusivity, solubilities, etc.); (b) fluid-rock interfacial tensions; (c) reaction rates associated with chemical processes at the mineral substrate; (d) the reservoir's permeability curves – with all of these parameters evaluated at the range of thermodynamic conditions found at the geological site.

RCGI Project number: 58

Recovery of alkali metals using electrodialysis cell: a computer fluid dynamics analysis

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Keywords: electrodialysis, computer fluid dynamics, metal recovery

Impact: Recently, there is a surge in demand for alkali metals for the energy transition process. However, the scarcity of this metals and the pollution associated with the mining process create problems specially for the environment. At the same time the oil and gas industry need to address the problem of the treatment of producer water, a waste brine present in oil and gas extraction. This saline solution is rich in alkali metals and can be a pollutant if discarded incorrectly.

Highlights: In this context, electrodialysis is process that can extract the metals from the producer water making it safe to discard to the environment and recover metals of economic importance. However, to properly use this system in oil platforms and others offshore installations more studies are need to optimize the process and increase its economic viability. Therefore, this work aims to simulate the an electrodialysis cell to optimize the metal recovery process from brine.

Abstract:
Currently, most metals are extracted by mining rocks. However, advances in water purification processes, such as desalination, have opened up the possibility of using brines and wastewater as raw materials sources. In addition to the treatment of effluents, these metals represent a high risk of contamination to the environment. Thus, the challenge of conserving these rare metals and metalloids together with environmental protection has strategically stimulated the need to extract and recover them from complex solutions. A technology studied for the recovery of metals from brines is electrodialysis. In this process, an electrolytic cell with membranes is used to produce two solutions, one concentrated and the other diluted. Thus, the concentration of metal ions occurs in a specific solution that can then be recovered via evaporation. This transport of ions is done by the electrical power supplied to the cell. Electrodialysis has proven its feasibility and high performance in the desalination of brackish water, desalination of amino acids and other solutions, effluent treatment, or industrial processes of recycling and salt production. Inside the electrodialysis separation plant is a conventional electrodialysis stack and cation and anion exchange membranes are placed alternately between the cathode and anode. When a potential difference is applied between these electrodes, the cations move towards the cathode and the anions towards the anode. Cations migrate through cation exchange membranes but are retained by anion exchange membranes. This project aims to perform computational analysis (computer fluid dynamics – CFD) of metal ion extraction systems from saline solutions to improve the performance of the system. Therefore, it will be evaluated different configurations and different parameters for the operation like: income concentration, electric potential, mixtures of salts and others. For the implementation of numerical models developed for electrodialysis, it will be used the software COMSOL, this program allows quick implementation of coupled multiphysics problems as is this case. Preliminary results, indicates the validity of the models proposed to study an electrodialysis cell. Besides, the numerical model of the process was created and validated in the COMSOL software.

RCGI Project number: 72

The role of the oxygen vacancies in the isobutene synthesis from ethanol

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Keywords: isobutene, ethanol, oxygen vacancies

Impact: The findings of this work pave the way for the generation of active and selective catalysts for the isobutene synthesis from ethanol.

Highlights: Oxygen vacancies play a key role in the isobutene synthesis from ethanol. Due to their basicity and redox properties, they promote all the steps of this cascade reaction, i.e., the oxidative dehydrogenation of ethanol, the oxidation of acetaldehyde to acetate species, the ketonization reaction, and also the aldol condensation of acetone which is the rate limiting step of the isobutene synthesis.

Abstract:
Isobutene is employed in the production of gasoline oxygenates, polymers, resins, and antioxidants. This work describes the isobutene synthesis from ethanol in only one step using a multifunctional catalyst. Five catalysts containing different amounts of Zn were prepared by impregnation employing m-ZrO2 and a Zn(NO3)2 aqueous solution. Catalytic tests were carried out using PFR-type reactor at mild conditions. The catalysts were characterized by ethanol-TPD, NH3-TPD, CO2-TPD, XPS, EPR, and XRD. A previous work of our group proposed the following mechanism for the synthesis of isobutene: firstly, acetaldehyde is generated from ethanol; then, this aldehyde is oxidized to acetate species which condense generating acetone; finally, this ketone undergo an aldol condensation, the intermediate species decompose generating isobutene and acetaldehyde. Analyzing the ethanol-TPD spectra it can be observed that acetaldehyde and H2O are simultaneously synthesized by oxidative dehydrogenation. These spectra also exhibit that isobutene formation is the rate limiting step (rls) of this cascade reaction. The XPS and EPR data show the presence of Zn+2 in the m-ZrO2 lattice, which creates pairs of oxygen vacancies and coordinatively unsaturated sites. These species exhibit redox properties which promote not only the acetaldehyde synthesis but also the acetate formation. The XRD and XPS results show the formation of a segregated ZnO phase for Zn concentration higher than 6%, which indicate a limitation of Zn2+ solubility in the m-ZrO2 lattice. A linear correlation between the amount of Zn on the m-ZrO2 surface (XPS) and the selectivity to isobutene was observed up to 6 at.% Zn, achieving the maximum selectivity of 44%. Some authors suggest that the □-H abstraction from acetaldehyde by strong basic sites is the rls of the aldol condensation. Oxygen vacancies are strong basic sites. Thus, it is possible to suggest that the aforementioned species are also associated with the formation of isobutene from acetone, the rls of this synthesis. Moreover, strong basic sites are also relevant for the acetate species condensation and the oxidative dehydrogenation of ethanol (□-H abstraction from the ethoxide species). Thus, due to their redox and basic properties, O vacancies are very relevant for all the steps of this cascade reaction. Understanding the behavior of this type of catalyst will allow its improvement, in addition to the proposition of new formulations.

RCGI Project number: 63

Catalytic conversion of CO2 to higher alcohols

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Keywords: Cu-Fe catalysts; MOFs; CO2 hydrogenation

Impact: There are a wide range of environmental, scientific and technological opportunities arising from the alcohols production from CO2. In this way, CuFe based catalysts are quite attractive, but also very challenging. Here, we use UiO-66 MOF catalysts for provide a foundation to develop CuFe catalysts for a selective CO2 conversion to alcohols, mainly C2+OH.

Highlights:
The UiO-66 was successfully synthesized and characterized.
UiO-66 catalyst have high crystallinity, well-defined morphology and high surface area even after the impregnation of Cu and iron nanoparticles.
Both XRD patterns and H2-TPR experiments suggests the Cu species interacted with Fe, possibly due the formation of an iron-copper alloy FeCu4.

Abstract:
The depletion of non-renewable energy sources and the constant fluctuations in the price of these reserves, along with the environmental problems caused by the massive amount of CO2 emitted into the atmosphere, have attracted much attention from society and aroused the urgency of seeking alternative sources of energy. Thus, the conversion of CO2 into fuels can contribute to solving these issues. Specifically, the synthesis of alcohols from carbon dioxide is quite attractive due to its wide range of applications. Cu-Fe compounds stand out among the catalysts that can be applied to the conversion of CO2 into products of interest. However, their synthesis needs to be linked to the need to comply with several challenges, mostly a products distribution in an undesirable proportion. In this way, the knowledge of the properties of the catalyst at the atomic level and the understanding of the mechanism of the reaction are essential to enhance the yields for CH3OH and C2+OH, and materials with nanometric structures have been promising for the issue. Along these lines, metalorganic structures (MOFs) have drawn intensive attention, mostly due to their highly ordered structure, tunable pore surfaces and high accessible surface area, which makes them very promising materials for heterogeneous catalysis, gas storage, controlled drug delivery vehicle, molecule separation, among others. In this work, CuFe/UiO-66-based catalysts were synthesized using hydrothermal and impregnation methods for application in the CO2 hydrogenation into alcohols. The powder X-ray diffraction (XRD), N2 sorption and transmission electron microscopy (TEM) characterizations show that the calcined UiO-66 support have high crystallinity, well-defined morphology and high surface area. Two samples, 25Cu/UiO-66 and 25Cu5Fe/UiO-66, were synthesized via the incipient-wetness impregnation method. The catalysts were characterized by XRD to determine the active phases crystalline structure, temperature-programmed reduction (H2 -TPR) to get the activation temperature, and N2 adsorption/desorption to measure the effect of Cu and Fe species in the specific surface area and porosity. Both XRD patterns and H2-TPR experiments suggests the Cu species interacted with Fe, possibly due the formation of an iron-copper alloy FeCu4. It is important to highlight that UiO-66-supported bimetallic Cu-Fe catalysts offer appealing opportunities for optimizing higher alcohols selectivity in CO2 hydrogenation. Also, this study open doors for new research directions and fulfills the potential of MOFs as a versatile and robust class of supports.

CO2 conversion into ethanol using catalyst based on combinations of rhenium and noble metals.

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Keywords: CO2 conversion, rhenium, noble metals.

Impact: The needs to reduce CO2 emissions into the atmosphere are high. Thus, effective measures to reduce CO2 are needed, developing economically viable strategies for capturing and valuing CO2. Ethanol is one of the most promising molecules among those that can be obtained directly from CO2. In this way, the development of catalytic processes that obtain ethanol from CO2 is an excellent strategy to combat the problem of climate change.

Highlights: Re with noble metals present great activit for conversion of CO2, at differnet conditions, where higher temperatures promote higher conversions, however, decrease the selectivity for alcohols due to the formation of methane. The 1/1 composition promoted greater selectivity for ethanol, with an ethanol/alcohol ratio of 10% for Ir-Re/TiO2.

Abstract:
Faced with the problem of climate change, the concept of carbon capture and use (CCU) has been globally researched in recent years as a strategy to mitigate CO2 emissions. Although there is no single solution to the problem, converting it into fuels and chemicals is an excellent strategy, and it can also give rise to a circular carbon economy, and with that, develop a new market segment. In this context, the conversion of CO2 into alcohols has been gaining prominence and has been studied by some authors, however, further studies are essential to develop an efficient and selective process to convert CO2, especially into ethanol, since the transformation of CO2 in these products is difficult due to the chemical CO2 inertia. Effective cleavage of the C=O bond and selective formation of the desired chemicals is still a challenge. Thus, the present work proposes to investigate catalysts based on noble metals such as rhenium (Re), iridium (Ir), palladium (Pd), gold (Au), ruthenium (Ru) and rhodium (Rh) in the conversion of CO2 into ethanol. The Ir-Re on titania, Re-Ru on titania and Pd-Re on silica catalysts were synthesized by wet impregnation and the Re-Au on titania and Re-Rh on zinc oxide catalysts were by deposition. The catalysts were tested under different conditions of temperature (200 250 °C) and composition of CO2: H2 (ratios of 1/1, 1/3 and 1/4), where they showed good activity for the formation of alcohols. Higher temperatures promote higher conversions, however, decrease the selectivity for alcohols due to the formation of methane. The 1/1 composition promoted greater selectivity for ethanol, with an ethanol/alcohol ratio of 10% for Ir-Re/TiO2.

RCGI Project number: 63

CO2 hydrogenation over Fe oxides catalyst: the effect of pretreatment synthesis on hydrocarbons selectivity

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Keywords: CO2 hydrogenation, Iron oxide, hydrocarbons

Impact: The abatement of CO2 has been received a considerable attention of industry and academic researchers. The CO2 hydrogenation to fuels and chemicals is an efficient route to control the CO2 emissions and decrease the dependence of fossil fuels. However, to achieve high activity and selectivity to higher hydrocarbons (C2+) is necessary the advance on development of design of catalysts and the reaction conditions.

Highlights:
The iron oxide catalysts are active to higher hydrocarbons synthesis from CO2 hydrogenation.
The pretreatment affects the reducibility and particle size of iron oxide.
The iron carbides phases are formed during reaction conditions.
The pretreatment affects the iron sites and thereby promote the hydrocarbons production.

Abstract:
The direct CO2 hydrogenation to higher hydrocarbons (HC) over bifunctional catalysts is usually reported, however a few studies investigated the selectivity and activity over Fe- monometallic catalysts. It is reported in literature that iron oxide phase is active for reverse water gas shift (RWGS) reaction, while the iron carbides is active for Fischer Tropsch synthesis (FTS) from CO hydrogenation. Although the nature of active site is still under discussion, we can expect a good hydrocarbon selectivity using bare iron catalysts under CO2 hydrogenation. In this work, the Fe3O4 nanoparticles about 10 nm were prepared by co-precipitation, then it followed by a calcination under air at different temperatures (400 – 800°C). The x-ray diffraction (XRD) showed the transformation of magnetite phase to hematite concomitantly the increase of iron oxide particle size with the increase of temperature of calcination. The temperature programed of reduction (TPR–H2) indicated the increase of temperature reduction of FexOy species with temperature of pretreatment. The performance of catalysts was evaluated under CO2 hydrogenation at 20 bar, 250-350°C, H2/CO2=3/1 in a fixed bed reactor. The samples achieve higher hydrocarbons selectivity (C2+) about 10-40% with CO2 conversion of 5-15% depending on the temperature of pretreatment. The calcination temperature affects the iron oxides nanoparticles size and their reducibility, that modified the distribution of CH4 and C2+ hydrocarbons. The characterization of spent catalysts revealed the formation of different species of iron (magnetite, maghemite, hematite, and iron carbides) during the CO2 hydrogenation conditions. The results suggest that presence of iron oxide concomitantly with iron carbide could be act as active phase on the promotion of the HC chain growth. Therefore, we demonstrated that the bare iron oxides catalysts synthesis method/ pretreatment (calcination) affects the ability to form the C-C bond at CO2 hydrogenation reaction. We are currently investigating the stability of these samples under the stream, and it´s promotion with alkaline metals.

RCGI Project number: 63

A Citizen Science Approach to improving public perception of low carbon society

Miguel Vera Moreno
Caetano Rodrigues Miranda

Keywords: Citizen Science; machine learning; Twitter

Impact: We study climate change, proposing citizen scientists contribute with evidence of climate change and environmental disaster. We hope that citizen scientists can help us better understand and propose solutions to climate change. Therefore, we can use the collected data to learn more about climate and environmental disasters. There is the success of projects in the world that use citizen science.

Highlights: Citizen science approach is designed for promote the interaction between research and the community to engage the public in science topics, for instance, climate change issues, greenhouse gases, and environmental disasters. Dissemination of the website and apps for the general public and post-processing Content production on the scientific and technological work developed by RCGI members.

Abstract:
Citizen science is an engaging strategy that enlists the public in gathering scientific information. Internet-based technologies have facilitated large numbers of volunteers to contribute in scientific projects. General public can contribute by collecting data and mapping how environments are evolving. It also can promote new interaction mechanisms and enable us to share and express ourselves as never before. This very conversational approach has contributed greatly 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. Social media have been extensively used in a broad range of fields for gathering real-time understanding of real-life behavior. However, there is little understanding of how social media may contribute to citizen science on the context of open data sources such as microblogging plataforms. One of most common is the Twitter, an open social media platform. Twitter supports such a conversational nature of discussion with large ammont and easy access for collecting data. This data can be a powerful source of information over a broad list of topics. Data then, can be analyzed to find trends over specific topics like climate change. At same time, it allows one to measure popular sentiment, obtain feedback on past decisions and also forstering trends. Only recently, climate change has received extensive attention from public opinion after being considered for decades as exclusive scientific debate. Governments and world-wide organizations such as the United Nations are working harder than ever on raising and maintaining public awareness toward this global issue. The aim of this project is to map the public perception of climate change and energy transition issues using twitter data.
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. The project also aims to promote the public engagement through citizen science plataform involving website, apps and post-processing content production on the scientific and technological work developed at RCGI.

RCGI Project number: 70

Science Diplomacy in the context of Climate Change: a bibliometric analysis

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Matheus Antônio de Souza Pereira - USP

Keywords: science diplomacy, innovation, bibliometric analysis

Impact: There has been an increase in the number of annual publications on science diplomacy since 2007. This results point to the importance of scientific diplomacy in the current political scenario.

Highlights:
This work conducted a bibliometric analysis of science diplomacy literature
- Number of publications have been increasing since 2007, reaching the current peak in 2021
- We constructed a keyword map to under the correlation of this term to other subjects
- Main connections of science diplomacy involve keywords related to health, environment and scientific cooperation

Abstract:
The project's advances focused on improving bibliometric analysis and literature review on Scientific Diplomacy topics. For theoretical foundation, the Scopus repository was used in May 2022, for a search with the exact term “Science Diplomacy”, from which a total of 259 works were obtained. Some publications with the highest number of citations were then selected. There has been an increase in the number of annual publications on the subject since 2007. The peak observed in 2020 and 2021 is a possible reflection of the concern of scientists during the Covid-19 pandemic. We observed that scientific diplomacy is related to several keyword groups, such as “technology”, “biotechnology” and “international cooperation”. In addition, a link with environmental issues can be observed in keywords: “environmental policy”, “sustainability” and “climate change”. Finally, we observe the connection of scientific diplomacy terms related to the history of its practice, such as “cold war”, as well as health issues “global health”, “pandemic”, and “covid-19”. This results point to the importance of scientific diplomacy in the current political scenario. Where countries need GHG reduction agreements to ensure climate security, and the reports, data and notes on the measures necessary to meet these goals are generated by scientists.

RCGI Project number: 70

Low-carbon technologies and their association with sustainable development goals

Mariana Ciotta, Celso Cachola, Alex Azevedo, Drielli Peyerl

Keywords: Low-Carbon Technologies, Sustainable Development Goals (SDGs), Decarbonization.

Impact: Maintaining alignment between low-carbon technologies and sustainable development goals is critical if the low-carbon economy is not to be built on developing problems. The implementation of decarbonization technologies is currently not often addressed from the SDG perspective in scientific publications. It is necessary to map these connections and networks in depth and define action plans.

Highlights: In this work, we seek to address how implementing low-carbon technologies is associated with sustainable development goals (SDGs). We use the Scopus database to understand how the scientific community publishes on these topics, seeking to map which SDGs are linked to the process of decarbonizing the economy and how this connection occurs. With this analysis, we aim to find out what the main gaps are so that it is possible to propose an action plan that considers effective measures to connect these universes of study.

Abstract:
Human development that considers climate issues as an urgent point of attention will have to take into account the development of low-carbon technologies. However, it is important that this process occurs in alignment with the sustainable development goals (SDGs) because the decarbonization of the economy cannot happen at the expense of other developing problems. In the case of this work, we chose to evaluate two study universes: carbon capture and storage (CCS) and bio-energy carbon capture utilization and storage (BECCUS). Starting from these two topics, we searched the Scopus database for academic papers to understand how these low-carbon solutions are associated with the SDGs and, more specifically, with which SDGs. In the Scopus database, 9 scientific articles address the issue of low-carbon technologies associated with the SDGs, and it is also possible to find 18 documents that deal with “CCS and SDG”, while no papers associating "BECCUS and SDGs" were found. However, the strength of the correlation of these themes is diverse and will be addressed in this work, specifically correlating which SDGs relate to which low-carbon technologies and in what ways. It is common for the topic of SDGs to be treated only as an a priori attraction of low-carbon technologies. Still, the alignment of these fields tends to be overlooked (or, more specifically, disconnected) in the evolution of decarbonization research. From this observation arises the analysis of gaps that need to be addressed and the proposition of ways to solve the problems investigated. We attempt to provide a methodology that enables a greater link between these themes: the SDGs must be an endless horizon in decarbonization planning, and the elaboration of scientific papers that consider this is an essential initial step.

RCGI Project number: 70

Improving the industrial ethanol fermentation using metabolomics and Maldi-TOF

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Keywords: Maldi-TOF; Fermentation; Metabolomics

Impact: This project provides an excelent opportunity to identify the main factors that determine the success of the fermentation process in the sugarcane industry, in Brazil. Bioethanol is produced in a very complex process where the conditions are poorly controlled, and contamination of the vascs are a routine problem. By using the Maldi-Tof tecnology it will be possible to identify the microbiota that causes major losses on yeast efficiency. Besides, using metabolomics methods it will be possible to understand the exchange of molecules between yeast and bacteria, and identify the best biomarkers that might be usefull to develop a control system for the fermentation processes. We expect that combining fast microbiota identification with biomarkers will result in lower losses of bioethanol due to contamination of the fermentation processes.

Highlights: The novelty of using metabolomics and Maldi-TOF to understand the complex process of bioethanol production in Brazil. This knowledge will provide the means to develop a better control system using biomarkers, biosensor, and machine learning to develop an independent control system of large scale fermentation. Antecipating the effects of contamination and interfering in advance to correct the problems, as soon as they start.

Abstract:
Currently, Brazil is the second largest producer of bioethanol in the world, becoming a world reference in sustainability. One of the main causes of this high productivity is the selection of S. cerevisiae strains adapted to the process. However, large-scale fermentation does not occur in an aseptic environment, providing the proliferation of various contaminating microorganisms that cause relevant losses to the process. In this way, the identification and quantification of contaminating microorganisms can help to minimize the losses of efficiency and productivity in industrial fermentation, providing intervention at the beginning of the infection, when it is still possible to control the process with the addition of antibiotics. The most used methods for identifying these microorganisms are biochemically or based on the DNA sequence, which are very time consuming, expensive and often lead to ambiguous results. Fermentation lasts for around 8-10 hours, with no time for real-time identification by conventional methods. Thus, a new approach is being developed in our laboratory, using the technology - MALDI-TOF-MS, a powerful tool for microbial identification, fast and with high sensitivity, allowing the identification of microorganisms almost instantly.
This project aims to adapt the MALDI-TOF-MS technology to the routine of first-generation (1G) ethanol production, using two of Raízen's plants as a model; Rafard Unity having a continuous feeding system of fermentation, and at Santa Helena unity, which has a fed batch fermentation. This methodology will also be used in the second-generation (2G) ethanol pilot plant, located at Usina Costa Pinto, in Piracicaba-SP. With this technology, we intend to monitor the contamination of fermentation vats

through biotyping and quantification of bacteria such as Lactobacillus spp, Acetobacter spp and other contaminating species most common in fermentation vats, as well as commercial and wild strains of S. cerevisiae. The MALDI-TOF-MS technology has been being improved in our laboratory, at the Genetics Department of ESALQ-USP, for about six years. Initially, we carried out a survey of the main microorganisms present in vats of two plants in Piracicaba-SP, during the 2015/16 harvest period (Bonatelli, et al., FEMS Microbiology Letters, 364, 2017). Based on the metagenomics technique, it was possible to identify the main species of contaminating microorganisms, with the genera Lactobacillus and Acetobacter appearing as the main contaminants. From this study, we obtained purified cultures derived from a single colony of each contaminating bacteria species. From this information, we built a database of mass spectra profiles of each species of bacteria, enabling their identification using the MALDI-TOF – MS technique. These mass spectra are then used as a reference for the search for biomarkers of each strain. Statistical classifier models were generated with the aid of Machine Learning techniques, making it possible to rank the most promising set of spectra as specific biomarkers for each data set. Based on this set of information and knowledge available in the laboratory, we are proposing to scale this technology to the industrial level, using the Raízen plant´s in Piracicaba and Rafard-SP as a model.

RCGI Project number: 75

Thermodynamic analysis of multistage carbon dioxide compressor: life cycle condition

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Keywords: multi stage compressor; energy consumption; lifetime cycle

Impact: Reduction in energy consumption and CO2 emissions

Highlights: Previous study shows power consumption reduction when pressure ratios are optimized;
* New model will be based on compressor map estimates;
* Compressor life cycle will be considered, with variations in mass flow, composition and anti-surge recirculation;

Abstract:
The petroleum industry uses supercritical CO2 compression systems to implement carbon capture and storage (CCS) and enhanced oil recovery (EOR) techniques. In both applications, the compression system is responsible for a high energy demand, totally justifying the investment in optimization of these compression systems. During the life cycle of the compression system, the variation in oil production imposes high variation in flow rate which demands one optimization routine that takes this variation into account. Usually, multistage centrifugal compressors are used in these compression systems and they are known to have a narrow operating range concerning flow rate. To deal with the variations in mass flow rate, the compression systems use recirculation through an anti-surge valve. This technique is effective in allowing operations at low flow rate conditions but impose extra energy consumption and reduced efficiency.
This work presents one model (under development) to support the specification of each compressor stage design point. The model will consider the energy consumption during the life cycle of the compression system in the determination of this optimum. Variations in mass flow rate, gas composition, stage efficiency and anti-surge recirculation are considered by the model procedures.

RCGI Project number: 77

STRUCTURAL, VIBRATION ANALYSES AND OPTIMIZATION OF CENTRIFUGAL COMPRESSORS FOR SUPERCRITICAL CO2 APPLICATIONS

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Keywords: centrifugal compressor, structural analysis, fluid-structural interaction

Impact: Emission of carbon dioxide (CO2) is one of the main causes of the greenhouse effect, its presence in the atmosphere largely increased in the current years. Thus, in addition to the direct reduction using new forms of energy, it is necessary to advance toward Carbon Capture, Storage, and Utilization (CCSU) technologies. The research focused on CCSU is expanding knowledge on the use of CO2 in a supercritical state (sCO2).

Highlights: With respect to centrifugal compressors, the use of sCO2 as a working fluid provides the construction of more compact structures, reducing the mass of the components as well as material costs. On the other hand, due to the high specific mass, the aerodynamic loads from the fluid-structural interaction have a greater amplitude, in addition, to directly affecting the impeller vibration modes, requiring careful studies regarding the structural failure modes and, therefore, modal analysis for resonance verification are essential to enable the structural integrity of the turbomachine and design components with long service life.

Abstract:
This work will present the current developments and next research steps regarding structural, modal vibration analysis, fluid structure interaction and optimization of centrifugal compressor impellers operating with CO2 in supercritical state.

RCGI Project number: 77

TOPOLOGY OPTIMIZATION OF COMPRESSIBLE SUBSONIC TURBULENT FLOW CONSIDERING FLUID-STRUCTURE INTERACTION

Emilio Carlos Nelli Silva, Renato Picelli, Cesar Kiyono, Luis Fernando Garcia Rodriguez, Carlos Okubo, Lucas Siqueira, Romulo Cortez, Felipe Maffei, Jurandir Yanagihara

Keywords: topology optimization, compressible flow, fluid-structure interaction

Impact: The coupling of fluid-structure interactions with the recently developed topology optimization method to get the adjoint system of the compressible turbulent regime for real gases could optimise the compressor rotors used in the Carbon Capture and Storage technology by reducing their energy consumption, improving the stiffness and avoiding resonance frequency.

Highlights: This work presents a topology optimization formulation for compressible turbulent subsonic flow designed for perfect and real gases, which gets the adjoint system through adjoint finite differences and an automatic differentiator approach. These methods are being coupled with an FSI study to avoid the resonance frequency and control the material stiffness in the rotor component.

Abstract:
The rotor of the compressor used in the carbon, capture and storage (CCS) compression system presents inefficiencies due to challenges related to the transport of supercritical CO2, which enhances hard modelling and characteristics of compressible turbulent flow such as large velocities, compressibility effects, rotational forces, turbulence phenomenon, temperature gradients, shock waves, real gas influence and vibrations that could lead to failures in the rotor design. Therefore, the flexible and robust topology optimization (T.O.) technique of fluid flow is being developed to deal with the mentioned challenges in a simultaneous optimization process. The T.O. can innovate fluid flow passages by changing the domain cells permeability through the characterisation of the fluid flow via the CFD modelling and the sensitivities calculation of a Lagrange system in a combined process. The fluid flow is modelled by the Favre Averaged NavierStokes (FANS) equations and the sensitivities calculation of the compressible adjoint system can be obtained by two differ ent methods considering the discrete adjoint approach: the adjoint finite difference method and the automatic differentiation tool. In the finite difference method, the adjoint model is built by adding a small perturbation in the state variables and calcul ating the residual between the original and perturbed system of equations. It has been developed and implemented with a finite element method discretization to treat compressible regime for perfect gases and the turbulence phenomenon is treated with the fr ozen turbulence approximation up to this day. The automatic differentiator approach considers the discrete forward equations and derives automatically the adjoint code via matrixial and symbolic manipulation using an automatic differentiator tool, and is d eveloped by combining the OpenFOAM and FEniCS software to deal with the compressible turbulent subsonic regime for real gases. In both schemes, the FSI analysis is coupled to avoid resonance frequency on the optimized rotor and consider the physical vibrat ion modes. Simultaneously, an FSI geometry trimming for the compressible regime, where the stress and natural frequencies are included as a constraint, and from the structural perspective, it is aimed to avoid resonance frequency by controlling the stiffne ss, efficiency, and volume of the optimized rotor. These approaches are being implemented for High Performance Computing (HPC), which makes possible the optimization of 3D complex domains .

RCGI Project number: 77

Topology Optimization of Fluid-Structure Interaction Problems Considering Natural Frequency Constraints

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Keywords: Topology Optimization, Vortex-Shedding, Vibration

Impact: The injection of gas mixtures in supercritical state into underground oil and gas reservoirs has been growing to increase the productivity of the reservoirs and capture the carbon emitted into the atmosphere. For this, the use of optimization techniques to improve the design and efficiency of these compressors to reduce energy consumption in these operations is of great importance.

Highlights:
- Inclusion of modal analysis and natural frequency sensitivities in the TOBS-GT method framework;
- Solving optimization problem of minimizing compliance subject to a natural frequency constraint without considering the volume constraint;
- Proposal of a methodology that indirectly allows to improve the design of structures subject to fluid induced vibrations using topology optimization;

Abstract:
This work is associated with the projects "Design of smart labyrinth seals for mitigation of GHG emissions in pneumatic machines" and “Design Optimization of Centrifugal Compressors for Supercritical Gas Mixtures”, from RCG2I. In both projects, one will work with rotating devices with narrow tolerances that can present wear problems due to excessive vibrations. From this, it is necessary to improve the design of these equipment in order to reduce the vibration levels of these equipment, moving their natural frequency away from the resonance conditions. In this context, this work addresses topology optimization of fluid-structure interaction (FSI) problems considering natural frequency constraints. The TOBS-GT technique is used as a method to separate the physics analysis and optimization grids. To observe the vortex shedding in the structure, a transient simulation is performed considering the incompressible laminar fluid flow. The structure is resolved using an elastic formulation with geometrical non-linearities to allow for large deformations. For topology optimization, the fluid flow is at steady-state and the structure is modeled considering small displacements. We solve a compliance minimization problem subject to a natural frequency constraint. The TOBS (Topology Optimization of Binary Structures) method is used to solve the optimization problem and find the new material distribution. The finite element method is used to solve the forward fluid-structure equations and the compliance sensitivities are calculated by automatic differentiation using COMSOL Multiphysics software. Natural frequency sensitivities are analytically derived and implemented in MATLAB. This methodology is an attempt to improve the design of structures subject to Flow-Induced Vibration (FIV). The procedure consists of moving away the natural frequency of the structure from the vortex-shedding frequency. Numerical examples show that the TOBS-GT method can be effectively applied to design 2D structures in FSI problems considering FIV maintaining the natural frequency in levels established in the optimization process and attenuating the levels of displacement at the analyzed points of the structure.

Understanding and optimizing the functioning of selected locally available oxygen carriers for Chemical Looping Combustion (CLC)

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Keywords: Chemical Looping Combustion, Carbon capture and storage technologies, oxygen carrier particles

Impact: Carbon Capture and Storage (CCS) has been a revolutionary proposal as an alternative technology to capture up to 100% of CO2 in fossil fuel burning processes, with low energy loss. In this context, the current work proposal is directed to the research of the CLC system, already in full development at the Laboratory of Thermal and Environmental Engineering (LETE) by prof. Fernando Sacomano and his team, mainly seeking to improve the system's methodologies.

Highlights: The capture and utilization of CO2 for producing commodity chemicals and fuels is one unique concept that can significantly contribute towards global clean energy initiatives. Chemical looping processes are promising on this regard and relies on the thermochemical (≥800 °C) uptake/release of oxygen by a metal oxide in a cyclic manner. The main objective of the CLC system is the transfer of atmospheric oxygen to the fuel through the active metal oxide, in order to avoid direct contact between the fuel and the air.

Abstract:
Chemical looping combustion (CLC) is more efficient than existing carbon capture technologies, since the energy lost in separation is negligible, NOx emissions are reduced inherently, and the carbon dioxide produced is pure enough to be sequestered immediately without the need for further expensive processing. This technology makes use of oxygen carriers, such as metal oxides that circulate between the fuel reactor, where they are reduced, and the air reactor, where they are re-oxidized. The selection criteria of the metal oxide include reaction rate, gas selectivity, and recyclability in multiple redox cycles, mechanical strength, cost, environmental impact and so on. Iron-based oxygen carrier is an attracting option due to its inherent characteristics and can be used in all chemical looping conversions mentioned above. Especially, the raw iron ores and some industrial wastes which contain iron oxides can be used as the oxygen carrier after some simple treatments. In this sense, the first step of this project consisted in the selection and characterization of naturally occurring ilmenite (FeTiO3) ores available in the Brazilian market. The selected particles were investigated regarding their composition, structure and morphology, under different conditions pertinent to the CLC process. Initial results (Figure 1) revealed rounded shaped particles of around 100 nm/diameter and its crystalline structure showed ilmenite as the main peak at 30Θ degrees based on X-ray diffractometry. The monitoring of mass loss or gain as a function of temperature was performed by thermogravimetric experiments in atmosphere of synthetic air, where the observed mass gains occurred due to ilmenite oxidations in which non-volatile oxides were formed. The next step consists on investigations of the mechanical stability, including safety and attrition of ilmenite after calcination.

RCGI Project number: 67

Structural Topology Optimization Including Smooth Boundaries Representation

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Keywords: Structural Topology Optimization, TOBS-GT, Smooth Geometry

Impact: Cycles operated with supercritical CO2 have received significant attention in recent decades in the field of renewable energies. As compressor efficiency plays an important role in the efficiency of the cycle as a whole, the development of optimized equipment can lead us to designs with better efficiency in their operation.

Highlights:
- Implementation of an algorithm for smoothing boundaries in structural topology optimization;
- Automatic smoothing of 3D geometries via Matlab;

Abstract:
This work is associated with the project “Design Optimization of Centrifugal Compressors for Supercritical Gas Mixtures”, from RCG2I. In this project, structural optimization will be carried out including fluid-structure interaction (FSI) with turbulent flow. One of the obstacles in the implementation of topology optimization methods in a FSI problem considering turbulence is the difficulty in converging the fluid flow solution. During the optimization steps, the optimizer removes and adds solid material in a fixed mesh, which can generate a rough (jagged) geometry. This condition leads to the phenomenon of boundary layer separation, causing the formation of vortices and instabilities that difficult the convergence of the computational fluid dynamic (CFD) analysis. To solve this problem, we developed a boundary smoothing procedure to be used during the optimization. Additional features of the algorithm include automatic trimming of 3D geometry and constraining the positions of mesh points at nodes where boundary conditions are applied. The (Topology Optimization of Binary Structures with Geometry Trimming) TOBS-GT is a method that benefits from the developed technique. In this method, sequential integer linear programming is employed to solve the optimization problem and find the new material distribution. We use COMSOL Multiphysics software to solve the physics via the Finite Element Method (FEM) and calculate sensitivities by automatic differentiation. We compare our method to previous literature results and related algorithms and prove that our smoothing procedure has potential to improve the appearance and performance of the resulting structural surface. For now, only single physics structural design examples are investigated. Expected future results include implementing the smoothed TOBS-GT method in the FSI framework.

RCGI Project number: 77

Topology optimization of non-isothermal PEM fuel cell cathode flow field

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Keywords: Topology optimization method; PEM fuel cell; Nonisothermal model;

Impact: The topology optimization method (TOM) has been widely applied to engineering problems over the past decades. Only two studies focused on applying TOM to design the flow field of fuel cells. However, they use a simplified model and lack experimental validation. This work expands the model by considering the heat transfer contribution in the model, as well as the comparison with an experimental fuel cell with a conventional flow field.

Highlights:
- A non-isothermal 3D PEM fuel cell is simulated.
- The results are compared to experimental data.
- A 2D simplification is used to model the cathode flow field.
- The flow field of 2D PEM fuel cell is designed using a topology optimization model.

Abstract:
Fuel cells are comprised of different components where flow fields play a significant role in their overall efficiency. The flow field design is responsible for most challenges in fuel cell operation, including inefficient gas distribution and degradation due to hot spots. The cathode flow field is of higher importance as the reaction is slower than the anode side. Also, it is on the cathode side that most of the heat is produced. Thus, the topology of the cathode flow field has a direct impact on the fuel cell performance and presents an opportunity for optimization. Topology Optimization Method (TOM) can be utilized to design the flow field channels in a way that maximizes a predefined objective function and creates non-intuitive topologies. The objectives of this work are: simulating a full-layered 3D non-isothermal PEM fuel cell, verifying the model against experimental data, reducing the 3D cathode side model to a 2D simulation, performing the topology optimization aiming to maximize the power generated, and finally comparing the serpentine and optimized flow fields in 3D. The model considers a non-isothermal PEM fuel cell with a 50 cm2 active area and a single-serpentine flow field modeled in three dimensions. The cathode and anode of the fuel cell consist of a bipolar plate (BPP), gas diffusion layer (GDL), and catalyst layer separated by a membrane. The simulation consists of a multiphysics problem with the contribution of mass, momentum, species, charge, and energy conservation equations. The 3D model is verified against experimental data in terms of polarization curve and temperature distribution. Next, the model dimension is reduced from 3D to 2D in order to reduce the computational cost and enable the use of topology optimization. Finally, a 3D fuel cell model with the optimized flow field is produced and the results are compared to the traditional serpentine flow field.

RCGI Project number: 83

MOF's to "Agrotechnology": CO2 Capture and Nutrients delivery

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Keywords: MOF; Soil Remineralization; Carbon Capture

Impact:

Ecosystems play an active role in the climate system, especially through their role in the carbon cycle, the water cycle and other biogeochemical cycles. Forest protection and restoration have received much attention for maintaining the planet's ecosystem balance and climate change mitigation. However, soil also plays a key ecosystem function and does not receive proper attention. Soil is a body in constant process evolution and acts as a water reservoirs, gases adsorption system, nutrients store, microorganisms warehouse and also provides support for plant growth and development. In this way, soil can integrate areas of environmental climate, biodiversity, food security and sustainability.

Along with continuous soil alteration processes, nanostructured minerals are formed, constituted mainly by metal oxides, which are responsible for several ecosystem functions in soil. The natural nanoparticles formation process, take place in a long time, approximately 300 years, to produce one centimeter (1.0 cm) of soil. These "natural nanoparticles", can vary according to the countries regions, environmental climate and geology. That different nanostructures can express to the soil different functions such as water absorption, acidity regulation and gases fixation. Recent studies, shows that increase global temperature can decrease of Hematite (Fe_2O_3), mineral that contributed to carbon storage, in amount 10%.

Soil remineralization, with attention to deficient minerals and biological digestion of these minerals to make them available for plant life is key in increasing soil carbon. Numerous studies have shown the capacity to increase soil carbon levels using rock powders in remineralization methods. This practice can increase the formation of new "natural nanoparticles" in a shorter period of time compared to the natural process, and contributes to the improvement of the soil's ecosystem functions, such as increasing nutrients viability, enabling water infiltration and greater gas storage.

Highlights:

Considering the benefits of adding powder minerals to soil, such as rock powders with particle size of many micrometers, we can anticipate that the utilization of "synthetic minerals", such as porous and high surface area micro/nano-structured materials, for the remineralization process in soils, will release their minerals more quickly to replenish soil ecosystem functions. Additionally, bacterial processing, known as assisted mineralization, can be used to delay nutritional elements release during population growth. An important prerequisite for this bacterial-assisted mineralization process is the solubility of an activation carbon source, responsible to stimulating soil microorganisms. Oxalate is a carbon source that plays an important role among microorganisms, soil and plants enabling nutrient chelation and increase their bioavailability. Consequently, oxalotrophic bacteria occur in almost any soil, they use oxalate as a carbon source for their metabolism, producing carbonates that are mineralized in the soil.

The hypothesis for this research project is that synthetic nanoparticles may improve soil ecosystem functions and CO_2 sequestration. This project has the following objectives: i) increase the soil's potential to store CO_2; ii) contribute to slowing down the biogeochemical cycles of N, S, C and H_2O, through the inclusion of nanoparticles; iii) assist resilience to external weather events, improving agricultural and environmental performance.

Abstract:

Cases developed by members of the São Paulo Environmental Agreement and published in United Nations Climate Change Conference of the Parties - 2021 (COP-26), indicate that natural nanoparticles and soil management, increase the concentration of carbon on average of 0.4 ton per hectare. Keeping this carbon into the soil of 25 thousand hectares is equivalent to avoid the emission of CO2 equivalent to 10 thousand tons the amount of gases emitted by 3,600 buses traveling on average of 15 thousand kilometers per month during one year, which require the plantation of approximately 73,000 tree seedlings or to have almost 40 hectares of “standing forest” to offset this emission.

Brazil has about 54 million of arable and productive land. Considering a scenario of implementation of the methodology of remineralization in only 1% of the cultivated areas with perennial crops, those that stay in the soil longer and then assist in the increase of the carbon permanence into the soil, we are referring to about 186 thousand hectares. Extrapolating the results of the case, considering only 50% of the efficiency of carbon permanence in the soil, it means an average increase of 0.2 t/carbon/ha into the 0 to 20 cm of soil layer instead of 0.4. Therefore, preserving only 1% of agricultural areas cultivated with perennials crops in Brazil, the amount of CO2 that would no longer be emitted owing to the degradation of carbon in the soil would equate to a fleet of about 26 thousand buses traveling on average of 15,000 miles per month for 1 year. In case of these CO2 values offset, it would be necessary to plant approximately 540,000 tree seedlings or have the equivalent of almost 300 hectares of “standing forest”.

In this way, this project select the Metal Organic Frameworks (MOF) using carboxylic linkers, like oxalates, to improve remineralization of soil and its ecosystem. The synthesis of these compounds is known and constitutes a class of materials with high porosity and structural chemical organization. MOFs can be synthesized to contain layers of metallic oxides (Fe, Mg, Zn, Al) and phosphoric oxides interconnected by oxalate, like organic linker's, forming an anionic framework that is neutralized by cationic guest residing inside the pores like ammonium molecules (NH4+) or potassium cations (K+). The MOF structure can be tuned to offer all elemental nutrients for accelerate soil remineralization process. The microbial consumption of the oxalate organic linker drives the collapse of the structure, thereby releasing the phosphate-metal from within and forming carbonate. The metallic oxides nanoparticles, formed after MOFs degradation, will interact with the phosphate and ammonium ions, helping their mobility and absorption by the plant roots.

The chemical structure of MOF's can be tailored depending on the type of soil and the type of crop, employing artificial intelligence methodologies, to generate valuable data for the development of innovative technologies for regenerative agriculture. The tailor-made MOF may contain oxalate derivate from CO2 in its structure that may decompose to form carbonates and mineral nanoparticles with the potential to change soil ecosystem functions and promote carbon dioxide capture.

RCGI Project number: 85

Computational study of homogeneous catalysts based on non-noble metals in the production of C2+ molecules using CO2 as the primary source of C1.

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Keywords: homogeneous catalysis; carbon dioxide hydrogenation, computational chemistry

Impact: Since the industrial revolution, the high rate of CO2 emission has become a global issue in view of its implications for climate and ecological change. Studying the transformation of CO2 into value-added products, appears as an attractive alternative, both for reducing the effects of global warming caused by the increase in the concentration of carbon dioxide, and for offering a solution to replace the use of fossil fuels.

Highlights: In view of the computational studies carried out, the homogeneous catalysts based on non-noble metals have revealed a high conversion potential in the hydrogenation reaction of carbon dioxide, forming several products (e.g. methanol, formic acid and formaldehyde), and some advances have already been seen in relation of C-C bonds formation, in respect of C2+ products production.
It was identified that the presence of electron-withdrawing substituents in bidentate ligands that are coordinated to the metallic center are more effective than electron-donating substituents. In addition, it was identified that there are no significant differences in the exchange of the phenanthroline ligand for bipyridine.

Abstract:
Carbon dioxide (CO2) is widely known as a gas that promotes the greenhouse effect, a phenomenon of natural origin and extremely important for the existence of life on Earth. However, with the increase in CO2 emissions since the industrial revolution, diferente pathways have been sought to use it as a raw material in the production of species that are less aggressive to the environment and/or that have added value. In this way, the area of catalysis has delved into the transformation of this abundant, renewable and non-toxic source of carbon. The homogeneous catalysts present a satisfactory performance in the catalytic hydrogenation of CO2, acting in milder conditions with relative selectivity. Although several studies have already successfully achieved the formation of C1 products (e.g. methanol and formic acid), there is high interest in C2+ products using CO2 as the primary source of C1. Therefore, the main objective of this project is to investigate, from a computational approach, the use of non-noble metal-based catalysts in the CO2 hydrogenation reaction, elucidating the possible catalytic mechanisms of the reaction and the most important steric and electronic factors. to obtain adequate reactivity and selectivity.

RCGI Project number: 63

Enhancing crop system models for C and N balances: long-term scenarios to improve sustainable agricultural management practices

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Keywords: food security; crop modelling; greenhouse gases

Impact: Long-term scenarios for sustainable agriculture management could contribute to soil carbon sequestration and consequently climate change mitigation.

Highlights:
- Carbon and nitrogen balance processes will be studied in this project;
- Crop modeling has great potential to be used as a tool for exploring efficient management strategies for GHG emissions reduction in agriculture;
-Sustainable agriculture practices could to contribute with sustainable intensification of agriculture in Brazil.

Abstract:
Soil organic matter is the largest pool of carbon in the biosphere. The knowledge of soil carbon balance could help to forecast the depletion of soil carbon stocks and carbon dioxide (CO2) efflux. The soil carbon balance is directly related to the nutrient supply in the soil, mainly the nitrogen that has importance in global food production, and its impact on the environment related to ammonia (NH3) volatilization. In order to meet the increasing demand for food, feed, fiber, and biofuel agriculture areas in Brazil have been expanding strongly in the last decade reaching areas with adverse soil and climatic conditions. The scarcity of available new arable land for production increase raises the importance of agricultural intensification by increasing crop yields. Brazil is one of the largest agricultural producers in the world and has been assumed as a key place for supplying the global future demand for food at reasonable prices. However, the issues of GHG emissions and climate change have put extra pressure on food production that will be addressed with agricultural management practices that add sustainability to the production process. In this direction, recent publications have shown the effect of agricultural soil management on carbon sequestration and reduction of ammonia volatilization under different environmental conditions. These researches could be improved by crop modeling, which has been well tested under temperate conditions, but little has been published dealing with carbon and nitrogen balance processes with data collected from well-designed experiments under tropical and sub-tropical conditions. Cropping System Model (CSM) can be used for simulating the effects of soil carbon and nitrogen balance in several crops. Our goal in this research project will use the crop models that compose Decision Support System for Agrotechnology Transfer (DSSAT) ecosystems, in conjunction with field data, to determine the impact of several agricultural managements on greenhouse gases (GHG) emissions reduction under different environments, water availability, soils, crops, tillage practices, and organic amendments; making it possible to generate results on a large scale in time and space. In this way, this project could to contribute the sustainable intensification of agriculture in Brazil, and help to the goals of GHG emissions reduction assumed by the country in the Paris Agreement.

RCGI Project number: 54

Introducing the Carbon Capture and Utilization (CCU)-RCGI Programme

Liane M. Rossi - IQ-USP

Keywords: CCU, Carbon dioxide, conversion

Impact: The CCU Programme goal is to create value from CO2 emissions through the design of integrated processes for carbon capture and conversion to tackle climate change. In this circular carbon economy concept, CO2 is considered a valuable C1 building block to CO2-derived chemicals, such as intermediates, monomers, and fuels.

Highlights: The use of the emitted CO2 in a valorization process towards third generation ethanol could not only contribute to increase ethanol production but also dramatically reduce the CO2 emissions associated with this industrial activity, while contributing for the modernization of Brazilian sugarcane distilleries by promoting their transformation into true biorefinery.

Abstract:
The CCU program goal to create value from CO2 emissions through its conversion is developed using different strategies from photocatalysis, electrocatalysis, bioconversion, heterogeneous catalysis and organic synthesis. CO2 is considered a valuable C1 building block to CO2-derived chemicals. Our focus on the production of higher alcohols will allow the production of third-generation ethanol. The expected results are listed below:

- Development of photocatalysts and photocatalytic process for the directly conversion of CO2 into valuable chemicals by artificial photosynthesis and green hydrogen via water splitting using direct sunlight and dual absorber semiconductor materials.
- Development of electrocatalytic process using tailored electrocatalysts, electrolytes, and interfaces, to enable the electrocatalytic reduction of CO2 to C2+ products, and of N2 to NH3, including their combination for obtaining urea.
- Development of biological processes for CO2 fixation and conversion into high added value bio-based products such as bioethanol, bio-hydrogen and biopolymers.
- Designing novel catalysts and processes to enhance the selectivity towards catalytic conversion of CO2 into higher alcohols
- Designing novel catalysts and processes towards valorization of CO2-derived chemicals via catalytic conversion into monomers
- Synthesis of bio-based monomers, such as polyols and isocyanates, and combine them to synthesize new polyurethanes from CO2-derived chemicals.
- Use computational tools to gain insight into the mechanism, to optimize and design processes for carbon capture, conversion and usage under operational conditions.

The commercial application of the developed technologies will depend on the maturity reached in the different conversion technologies and may need to be further evaluated on pilot scale. Moreover, quantification of environmental benefits can be challenging and requires a comprehensive life-cycle assessment as well as understanding of market dynamics to help the definition of future policy and investment decisions. The technology may have a straightforward commercial application is the Brazilian bioethanol industry, since it is a sustainable source of heat and power and of a clean CO2 from fermentation. A tremendous potential can be explored if this Program develops an efficient and selective process to convert CO2 in third generation ethanol, which could increase the productivity of the existing bioethanol refineries. The use of the emitted CO2 in a valorization process towards ethanol could not only contribute to increase ethanol production but also dramatically reduce the CO2 emissions associated with this industrial activity, while contributing for the modernization of Brazilian sugarcane distilleries by promoting their transformation into true biorefinery, producing CO2-derived ethanol, and ethanol-derived monomers.

Rhenium-based catalysts for the conversion of CO2 to higher alcohols

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Keywords: CO2 hydrogenation, rhenium, supercritical

Impact: Towards one step conversion of CO2 to higher alcohols by heterogeneous catalysis

Highlights: Catalysts with a combination of rhenium and non-noble metals for the hydrogenation of CO2 to higher alcohols in supercritical conditions

Abstract:
A wide variety of products can be obtained from CO2, such as organic or inorganic carbonates, amides, urea, salicylic acid, synthesis gas, hydrocarbons and fuel alcohols. Due to a growing concern about climate change and the fluctuation of oil prices, more and more efforts are directed to make synthetic fuels a reality.
The thermodynamic stability of CO2 makes its hydrogenation to chemicals and fuels challenging, yet exciting and promising. Most publications on the synthesis of alcohols from CO2 focus on the production of methanol since higher alcohols are not attainable in large quantities. However, higher alcohols are also desirable – for example, in combustion engines, their higher octane ratings lead to lower emissions of ozone, NOx, CO, and volatile aromatic compounds. Therefore, the development of active catalysts in the direct hydrogenation of CO2 to higher alcohols is necessary.
In hydrogenation catalysis, rhenium has been recognized for its remarkable activity and selectivity in converting carboxylic acids to alcohols, and its lower susceptibility to poisoning and catalyst deactivation. A rhenium-based catalyst was also reported by our group to efficiently catalyze the conversion of CO2 to methanol. CO2 can adsorb and interact on the surface of metal oxides in different ways during hydrogenation reactions, leading to different intermediates and products. These surface species can react with protons, hydrides, and hydroxyls, forming products that include formic acid, formaldehyde, methanol, carbon monoxide, and methane. If the catalytic surface also contains an active site able to catalyze the carbon-carbon coupling in adsorbed species, C2+ chain products can be obtained. The functionality of the obtained product (i.e. hydrocarbon, alcohol) is also defined by the interaction of the intermediates with the catalyst.
In this project, a catalyst for the conversion of CO2 to higher alcohols at high pressure is under development. The catalyst compositions studied so far contain a combination of two or more active metals, starting with rhenium, which has already shown good results in similar reactions, and a non-noble metal is added. For instance, Na, K, Fe, Zn, or Cu, can be combined with rhenium and create multifunctional catalytic active sites. The active metals are supported in materials developed with the focus on favoring the C-C coupling, in order to grow the carbon chain and enable the production of higher alcohols.

RCGI Project number: 63

DFT Simulation of the CO2 Reduction Mechanism on the Mixed-Oxide Catalysts

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Keywords: CO2 hydrogenation, ethanol, DFT

Impact: Overall, the theoretical results are related to building and optimization of the perfect AlO2 and LaO-terminated LaAlO3 (001) surfaces and with the presence of Al, O, and La vacancies. In total, six catalyst models were found. The goal is simulating the CO2 adsorption and conversion through a configuration-driven mechanism. The conversion to the CH3CH2OH and H2O molecules will be simulated through the most favorable LaAlO3 (001) surface. Furthermore, the steps of the catalyzed reaction of hydrogenation of CO2 into ethanol may depend on surface defects, supporting the experimental results. Therefore, the influence of the vacancies will be evaluated in order to decrease the kinetic barrier.

Highlights:

Electronic properties were computed in the complex LaAlO3(001) catalyst surface

The CO2 conversion into ethanol could be significant on the LaAlO3(001) catalyst surface

Aluminum sites are catalytic sites more selective for adsorption of CO2

Abstract:
Due to the emissions of dioxide of carbon (CO2) from automotive and industrial exhaust, the main interest of this project is related to catalytic decomposition of CO2 that leads to production of higher-value products for clean air, electrochemical energy storage applications and renewable energy. Accordingly, the mixed oxides of perovskites (MOPs) are catalysts used in the CO2 reduction due to their low cost, earth abundance and to work in complex environments. However, the conversion of CO2 to in gases less harmful to the environment depends on the understanding of the complex ion exchanges and defects present on the surface of the MOPs and how these changes lead to the formation of intermediates in the CO2 conversion mechanism to produce ethanol, for example. This project aims to compute, by first principles methods, the different structures of the mixed-oxide of LaBO3 with substitutions by different transition metals in the B-position, the energy of formation of oxygen vacancies and in the B-position, and the kinetic energy barriers in the CO2 reduction mechanism and subsequent ethanol production. Therefore, it is intended to obtain with precision the main interactions on the catalyst surface. The main signatures in the interactions will also be obtained via simulation spectroscopic signatures by the solid state nuclear magnetic resonance (SS-NMR), making possible a theoretical-experimental collaboration. In addition, this catalytic study is very important not only in the context of greenhouse degradation, but also to favour cooperation between chemists, physicists and material scientists. As perspectives, the results of this project can be used to improve

high-throughput calculations based on calculations of first principles of properties that involve changes in the composition of materials with the ABO3 structure and in the types of degraded gases. This expressive set of data is essential for machine learning algorithms to predict new nanocomposites for the degradation of greenhouse gases.

RCGI Project number: 63

Investigating the perfomance of molybdenum catalysts in the CO2 hydrogenation for higher alcohols production

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Keywords: CO2 hydrogenation; higher alcohols; molybdenum

Impact: This research has excellent application perspectives for the ethanol chemical industry in Brazil. As a consequence, this research can promote the expansion of the ethanol market, improve technologies enabling cost reduction, contribute to the reduction of our dependence on the depletion of fossil resources, and bring environmental benefits due to the mitigation of CO2 emissions.

Highlights: The addition of potassium and a second metal, especially copper, enhanced of formation intermediates in the CO2 hydrogenation highlighting the potential for the application of these materials to produce higher alcohols.

Abstract:
Brazil is the world's second-largest ethanol producer, but the CO2 emitted during fermentation and the burning of sugarcane bagasse ends up in the atmosphere. The conversion of CO2 from sugarcane ethanol refineries into chemicals, for example, methanol, ethanol, acetic acid, is an opportunity to enhance and diversify Brazil's chemical industry. This process of direct conversion of CO2 to higher alcohols is still quite challenging due to the complexity of the possible reaction routes which depends on the operational conditions and the catalyst employed. Thus, for the synthesis of C2+ alcohols, the formation of C-C bonds on the catalyst surface before its hydrogenation and desorption is crucial. For that, molybdenum based-catalyst has been highlighted as a promising catalyst for alcohol synthesis since 1980. Its application has been investigated mainly in CO hydrogenation reactions using metallic Mo, MoO3, MoS2, β-Mo2C and MoP. Specifically, molybdenum-based catalyst has high sulfur resistance, low carbon deposition that provides sintering resistance, enhancement of the linear alcohol formation and low cost compared to other metals. However, the performance of Mo catalysts in CO2 hydrogenation to higher alcohols has not been explored so far. Some intrinsic limitations are associated with this reaction, such as the complexity of the possible reaction routes that depend on the operational conditions and the catalyst employed and the control of the selectivity. Thereby, the addition of basic promoters and a second active phase can overcome these limitations in molybdenum-based catalysts. Here, potassium was selected as a basic promoter owing to the suppression of H2 activation, which inhibits the alkylation reaction. In addition, copper and iron were selected as second active phase in order to increase the CO2 activation and CO/CH3OH production as well as C-C coupling to increase the hydrocarbon chain. Therefore, a deep understanding of the performance of these catalyst on CO2 hydrogenation has been explored at 300 ºC and 20 bar. The materials were synthesized by sol-gel method and calcined at 400 °C under static air for 3 hours. The unpromoted catalyst only produces CH4 and CO whilst the promoted catalysts showed mainly CH3OH and CO with the Cu-containing catalyst having the highest selectivity towards methanol. These previous results highlight a potential of these catalysts for higher alcohol production since both methanol and carbon monoxide are intermediates of the reaction mechanism. Therefore, the synthesis method and reaction conditions will be improved to increase the activity of the catalyst and optimize the selectivity towards higher alcohols, especially ethanol.

RCGI Project number: 63

A machine learning model for adsorption energies of chemical species applied to CO2 electroreduction

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Keywords: Machine learning, CO2 electroreduction, electrocatalyst

Impact: A significant contribution of this work lies in the fact that, with machine learning models, it is possible to obtain adsorption energies quickly and with a low computational cost, allowing a fast screening of materials. Furthermore, we can predict adsorption energies for ionic species on metallic surfaces, which is unfeasible to obtain directly through first-principles calculations.

Highlights:

- Machine Learning Model construction for CO2 electroreduction.
- Adsorption energy predictions on FCC transition metal surfaces.
- Adsorption energy predictions of charged chemical species.
- Determination of atomic periodic properties that most influence adsorption.
- Control of products generated from the electro-reduction of CO2.
- Tool for sorting materials optimizing selectivity in electrocatalysis.

Abstract:
The electrochemical reduction of carbon dioxide (CO2), a primary contributor to global climate change, is a necessary process that has been studied extensively. A key technology challenge needed to enable such a process to be done cost-effectively is to understand the potential of CO2 reduction electrodes better. Understanding the behaviour of metallic catalysts surfaces systems is fundamental to optimizing and controlling the CO2 electroreduction process.
In this work, we used machine learning methods to obtain adsorption energies of different chemical species on transition metal catalysts. Were considered the (100), (111), and (211) FCC surfaces of transition metals, and we also included the Pb. We implemented four machine learning models using information in databases containing adsorption energies obtained via first-principles calculations and useful libraries to represent the interaction between the adsorbate and the catalyst. Furthermore, we determined from these models the adsorption energy of CO, CO2, and CO2-• radical anion.
In a broader context, our results showed the robustness of machine learning models and the ability of these methods to speed up the screening materials to specific goals at a low computational cost. We emphasize the capability of our model to predict the adsorption energy of ions on metallic surfaces. It has a special significance due to the difficulty of calculating the correct energy for charged systems by traditional atomistic simulations.

RCGI Project number: 63

Synthesis and characterization of nanostructured materials for application in nanofiltration membranes

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Keywords: Nanofiltration; ZIF-8; Alkali metals

Impact: Oil & gas production water presents considerable contents of several ions. Among them, Li+ is in high demand in the Li-battery market, especially in reducing energy transition. Here we investigate different nanomaterials that can be employed in developing nanofiltration membranes to separate Li+ from O&G production water to increase the separation process's efficiency.

Highlights:

- Zeolitic Imidazolate Frameworks in sodalite structure (ZIF-sod) present pores with dimensions similar to the hydration radius of ions.
- Pore dimensions can be tuned according to the metal used in the structure of the ZIF analog.
- ZIF materials will be anchored in a modified polymer containing imidazolate groups.

Abstract:
Three different representatives of the ZIF-sod, containing Zn, Co, and Cd, were synthesized using the solvothermal route. The samples were named ZIF-Zn, ZIF-Co, and ZIF-Cd. A proportion of 8:1 of 2-methylimidazole: metal ion was employed in all syntheses. The reaction was carried out for 24 h at 130 ºC. The resulting solid was removed from the reactor and washed with water. The resulting suspension was left to decant overnight, forming larger agglomerates that allowed for filtration. After filtering, the solids were kept to dry in the oven for 24 hours. The synthesis through solvothermal methods has shown to be easy, and although it might present some impurities, it was possible to prepare the ZIF analogs containing Co, Zn, and Cd. The formation of the crystal structure was confirmed using XRD, with reactions with Co and Zn occurring readily, while the one with Cd has shown the need for a small amount of Et3N to be auxiliary in the mechanism. The absorption spectra of the samples were also acquired, showing characteristics of bands concerning the complexation of the metals with 2-methylimidazole. These values are in the wide range reported in the literature, varying from 4.7 eV - 5.1 eV for the ZIF-Zn - Eg, - 1.67 -1.98 eV for Eg1, 3.65 eV for Eg2, and 4.37 eV for the ZIF-Cd - Eg. The materials were also tested over their thermal stability through thermogravimetric analysis, showing that ZIF-Zn has higher toughness (400 oC) when compared to ZIF-Co (330 oC) and ZIF-Cd (180 oC). The results were compared with simulation data to increase the understanding of these materials, and the accuracy of the functional and force field used in the DFT calculations and MD simulations, respectively. Our next steps, which have already been implemented, are: 1) to measure the surface area of the ZIF-sod members, 2) to modify a polymer structure with terminal imidazolate groups, and 3) to force the growth of ZIF-sod structures to evaluate the structural changes on the material by XPS and FTIR. The final active membrane will be composed of this new Polymer/ZIF structure. This final topology will result from the processability associated with polymers, the porous characteristics of ZIF-sod structures, and the polymer crosslink brought by the insertion of the imidazolate functional group of the polymer in ZIF-sod structures.

RCGI Project number: 72

Electrochemical Technologies for Direct Lithium Extraction from Geothermal Sources and their Industrial Processes

Andressa Mota-Lima

Keywords: Lithium recovery, baterry electrode, plasma electrolysis

Impact: Electricity-based technologies for lithium recovery have the highest selectivity among other tecnologies, over reduces the overall number of industrial steps, operate with renewable energy, whether wind or solar, and can be fitted in any remote spot for treating either produced water or brine.

Highlights:
1 - There are two major electricity-based technologies : (a) plasma electrolysis and (b) Electrochemical ionic pumping (Battery-based electrodes).
2 - Both technologies enable a reduced number of steps in the industrial process and a lesser costly industrial production
3 - Plasma electrolysis enables the decrepitation of either salts or hydroxides; however its TRL is 1.
3 - Battery-based electrodes enables recover ultra-pure Lithium in two steps; and its TRL is 9.

Abstract:
Since 2017, several endeavors at the Qinghai salt lake deposit in China (Grant, 2020) have popped out due to the increasing request for high Lithium supply by the battery market that is currently expanding due to the global quest for renewable-based energy sources. According to Grant (2020), the current set of technologies used for Direct Lithium Extraction (DLE) includes (1) membranes, (2) adsorbents, (3) ion exchange, and (4) solvent extraction. All these technologies are of high TLR (Technology Readiness Level); however, such ordinary technologies deliver a salty medium (brine) effluent enriched with Lithium, needing several steps of downstream purification. Contrariwise, the electrochemical-based technologies exhibit higher selectivity toward Lithium, meaning a reduced number of steps in the final industrial process and a lesser costly industrial production. This talk presents the benefits of using electrochemical-based technologies and their possible industrial processes. Two electrochemical technologies are highlighted: the electrochemical ion pumping based on the lithium, potassium, and sodium battery-like electrodes and the cold plasma at the solid-liquid interface (or Plasma Electrolysis). After that, some industrial processes of lithium recovery containing less than three steps, all environmental friends, are presented. Finally, as much as exciting endeavors, the DLE community is invited to engage in such DLE challenges questing for disruptive advances.

Reference
Grant, A., 2020. From Catamarca to Qinghai: The Commercial Scale Direct Lithium Extraction Operations. Jade Cove Partners.

RCGI Project number: 72

LCA study of the uses of vinasse produced in the sugar-energy sector

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Keywords: LCA, vinasse, sugar-energy sector

Impact: This work may contribute to the identification and quantification of the impacts involved in the uses of vinasse generated in the sugar-energy sector, through LCA studies of different scenarios: in natura vinasse, biodigested and concentrated vinasse and biodigested vinasse together with filter cake (process of codigestion) and concentrated.

Highlights:
LCA of current uses of vinasse (fertigation, biodigestion, co-digestion);
LCA of the vinasse electrolytic concentrator, to be developed in the laboratory;
Potential environmental impacts associated with current uses of vinasse versus the use of vinasse electrolytic concentrator;
Dissemination of results in Workshops and publication of technical articles.

Abstract:
The use of vinasse to fertigate sugarcane fields has been the solution used by sugarcane mills to allocate the huge volume of this by-product of ethanol production. Vinasse has an important content of potassium and other nutrients, which allow an increase in sugarcane production per hectare, in addition to allowing a reduction in fertilizer consumption. By taking advantage of the vinasse in the fertigation of the sugarcane crop, it avoids its disposal in water bodies with resulting environmental impacts. On the other hand, the practice of fertigation with vinasse can cause soil salinization and contamination of underground aquifers, if the applied dosage is not in accordance with the type of soil and the variety of sugarcane.

Vinasse fertigation has a high potential for emission of greenhouse gases (GHG), including methane (CH_4) and nitrous oxide (N_2O). These emissions are produced due to the important content of organic matter and nitrogen present in vinasse. The decomposition of organic matter under anaerobic conditions, that is, without the presence of oxygen, emits methane during storage and transport. To minimize these negative effects of the application of vinasse in the soil on GHG emissions, it is recommended to develop better practices for the management of this residue. As a possible solution to these emissions, the biodigestion of vinasse stands out, which in addition to reducing the organic load present in the vinasse, also enables the capture and use of the biogas produced in the process, mitigating methane emissions into the atmosphere.

The possibility of integrating the anaerobic digestion of vinasse with subsequent concentration is also considered, thus allowing to solve important problems in its disposal. On the one hand, the huge volume and problems associated with its transport are eliminated; and on the other hand, it enables the energy use of biogas, both to replace fossil fuels and to supply part of the energy used in the vinasse concentration process.

In view of the above, this research project aims at the LCA of the uses of vinasse (fertigation, biodigestion of vinasse and co-digestion of vinasse and filter trot), as well as the elaboration of an LCA study of the vinasse electrolytic concentrator, developed in the laboratory within the scope of the project 56. The LCA studies will allow the identification and quantification of the impacts involved in the uses of vinasse generated in the sugar-energy sector.

RCGI Project number: 56

CO2 CAPTURE POTENTIAL IN THE SUGAR AND ETHANOL SECTOR IN BRAZIL AND SÃO PAULO STATE

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Suani Teixeira Coelho - IEE/USP
Colombo Celso Gaeta Tassinari - IEE/USP

Keywords: BECCS ; Climate mitigation; sugarcane

Impact: It is expected with the disaggregated results and the geological studies to identify the storage potential and the closest location for this storage.
It is expected that with the results the public policies will be elaborated and implemented so that BECCS is a reality in Brazil.
Evaluation of the implementation of carbon capture technologies in the process of anaerobic digestion of vinasse and filter cake and in the end uses of the produced biogas

Highlights: Determines the full mitigation potential of this BECCS technology in Brazil and São Paulo State.
Demonstrates the importance of sugarcane based bioenergy carbon capture and storage(BECCS).
Evaluates BECCS based on emissions from sugar fermentation and bagasse combustion.
Combining bioethanol production with CCS

Abstract:
Brazilian commitments at the Paris agreement, Bioenergy systems with carbon capture and storage (BECCS) are technologies that combine energy production from biomass with carbon capture and storage. These systems are essential to achieve the CO2 emission targets assumed by the signatory countries of the Paris Agreement not only by reducing CO2 emissions into the atmosphere, but also by removing it from the environment.
Brazil, as the world's biggest producer of sugarcane and ethanol, it has an important contribution to the reduction of global CO2 emissions and also to its removal from the atmosphere. In the 2020/21 harvest, according to CONAB - COMPANHIA NACIONAL DE ABASTCIMENTO- Brazil produced 654.5 million tons of sugarcane, of which 300 millions were destined for the production of 41.2 millions tons of sugar and the remainder, 354.5 millions tons, destined for the production 29.7 billions liters of ethanol.
Also, according to CONAB, the Center-South region of Brazil was responsible for approximately 90% of the ethanol and sugar in the 2020/21 harvest, with emphasis on the State of São Paulo, whose sugarcane milling in this harvest was 354.3 millions tons which were used to produce 14.39 billions liters of ethanol and 26.1 millions tons of sugar.
Based on production data for the 2020/21 harvest was estimated the theoretical potential for capturing CO2 in the Brazilian and São Paulo sugar-energy sector. The results show that the theoretical potential for CO2 capture for Brazil due to bagasse burning and fermentation process are respectively 242.16 and 22.57 millions tons of CO2. For the State of São Paulo, also for the burning of bagasse and the fermentation process, these values are respectively 131.09 and 10.94 millions tons of CO2.
For the calculations were used the values of sugarcane milling, ethanol production and CO2 factors for fermentation process and bagasse burning. It was also assumed that the CO2 generation factors are, respectively, 0.76 kg of CO2 per liter of ethanol and 0.37 tons of CO2 per ton of sugarcane milling, considering that all the bagasse produced is burned.

The magnitude of these numbers places the Brazilian sugar and ethanol sector, in especially the São Paulo sector, as the economic sector with the greatest potential for carbon capture and storage. Because that, within the scope of Project 58 (Applied assessment for the potential of BECCS in Paraná sedimentary basin in Brazil - Bioenergy Energy with Carbon Capture and Storage Program) the technical potential for capturing and storing CO2 emissions generated in the fermentation process and burning of bagasse is being estimated, in disaggregated form by sugar and alcohol plant.
Considering the perspective of using filter cake and vinasse for biogas production, CO2 emissions are also being estimated for each plant, considering the final use of biogas for generating electricity or producing biomethane. The use of these residues for biogas production will enable the capture of significant amounts of CO2.

RCGI Project number: 58

Molecular Simulations of Boric Acid Filtration by Carbon Structures

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Keywords: Boron filtration, Molecular Simulations, DFT calculations

Impact: This research explored how adequate the current descriptions of the interaction between boric acid and graphene in molecular simulations are. The results indicate that they are not adequate. To surpass this limitation, a new set of Lennard-Jones potential parameters has been proposed, which showed good agreement with DFT calculations. Its use should improve the quality of simulations of boric acid filtration.

Highlights: Boric acid shows relatively stronger adsorption energy toward graphene

- Loretz-Berthelot approximation underestimates the interaction between boric acid and graphene
- A new Lennard-Jones force field is proposed to obtain a better description between boric acid molecules and graphene in a good agreement to DFT calculations

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 healthy and agricultural consumption. Graphene is a promising material for filtration due to good mechanical properties and chemical stability. To investigate boric acid filtration through graphene by molecular simulations, 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. This observation suggests 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 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.

References: [1] -

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ABSTRACTS OF POSTER SESSIONS

Energy Transition
RESEARCH & INNOVATION

Avaliação do potencial de armazenamento geológico de CO2 na ocorrência de gás de Cuiabá Paulista, Bacia do Paraná, através de modelagem geológica implícita 3D

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Keywords: Armazenamento Geológico de CO2, Bacia do Paraná: Modelagem Implícita 3D

Impact: O projeto poderá indicar um sumidouro geológico de CO2 em uma das maiores concentrações de usinas de etanol e de fontes emissoras estacionárias do país, contribuindo assim para redução de emissões totais de dióxido de carbono.

Highlights: As formações geológicas da Bacia do Paraná na região sudeste apresentam potenciais pares de rochas selante-reservatório com favorabilidade para armazenamento de CO2.
A avaliação da ocorrência de gás de Cuiabá Paulista pode indicar uma possível aplicação de recuperação avançada de gás conjuntamente com armazenamento geológico de CO2.

Abstract:
A tecnologia CCS (Carbon Capture and Storage) é formada por uma série de etapas Integradas que tem por objetivo evitar a liberação de gás carbônico (CO2) na atmosfera, compreendendo desde a captura e transporte até a injeção e armazenamento de dióxido de carbono (CO2) em formações geológicas profundas. Atualmente a utilização da tecnologia CCS é de extrema importância, tendo em vista o atual cenário mundial de aumento gradativo nas emissões dos gases do efeito estufa. A aplicação de CCS está alinhada com a disseminação das metas de redução de emissão de carbono internacionais, como o acordo de Paris, que visam limitar o aquecimento médio da atmosfera a 1,5°C. A modelagem geológica representa uma das fases mais importantes no estudo de possíveis reservatórios de CO2 por determinar o volume de gás a ser armazenado. A região Sudeste do Brasil, onde está localizada a área de estudo, contempla rochas vulcânicas e sedimentares de formações Paleozóicas e Mesozóicas da Bacia do Paraná. Trata-se uma localização promissora, por estar próximo de uma das maiores concentração concentrações de usinas de etanol e de fontes estacionárias emissoras de CO2 do Brasil. As principais ocorrências de gás conhecidas na Bacia do Paraná são definidas por sistemas de pares de rocha reservatório-selante, formados pelos arenitos do Grupo Itararé e pelas soleiras de diabásio da Formação Serra Geral, respectivamente. Em Cuiabá Paulista, oeste do estado de São Paulo, o Grupo Itararé é subdividido em 3 formações (Taciba, Campo Mourão e Lagoa Azul). O projeto busca fornecer as bases geológicas para estudos futuros de avaliação econômica considerando o armazenamento geológico de CO2 conjuntamente com a produção de gás. O objetivo geral é avaliar parâmetros geológicos básicos para armazenamento de CO2 e gerar um modelo estratigráfico 3D. Mais especificamente, o trabalho visa analisar os dados litológicos e petrofísicos de poços de sondagem enfocando o Grupo Itararé, no que se refere à sua estratigrafia através de uma subdivisão em eletrofácies definindo pares de rochas reservatório-selante de melhor potencial e, por fim, calcular a capacidade teórica de armazenamento de CO2.

RCGI Project number: 36

Evaluation of microbial fuel cell for electricity generation from niobium-modified electrodes

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Keywords: Biocathode, Vinasse e Modified Electrodes

Impact: This project aims to investigate the effect of doping activated carbon at different concentrations of niobium, which is used with the electrode in the microbial fuel cell system. Niobium is a semiconductor and Brazil holds more than 90% of the world's exploitable niobium reserves. With this it is expected to optimize the operation of the MFC, since the electrode material is a determining factor, influencing the power density of the system. Using activated carbon, which is a three-dimensional electrode doped with niobium, aims to reduce the losses associated with electron transfers.

Highlights: Obtaining a mature inoculum with more than 400 days in operation and organic matter removal above 75%.
This project is in the prototyping stage, but we have already obtained positive sealing results, the next step is to finalize the assembly and put the reactors into operation.

Abstract:
"One of the great current challenges is the development of technologies that seek to supply the energy demand and the treatment of wastewater. In this context, microbial fuel cells (MFC) present themselves as a promising technology, as they allow the conversion of chemical energy, from different substrates, to electrical energy.
However, this process has some limitations and challenges that seek to improve and increase energy and treatment efficiency. This work aims to evaluate the use of carbon-based electrodes chemically modified with niobium at 5, 25 and 50% by weight, in energy generation, organic matter removal and autotrophic denitrification in the treatment of synthetic vinasse. MFCs are of the dual chamber type. The study is divided into 4 operational phases, being Phase 1: Prototyping, Phase 2: Inoculation and Adaptation, Phase 3: Coupling of the reactors, Phase 4: evaluation of efficiency with the increase of organic load. The efficiency of the system will be evaluated by physical-chemical and electrochemical parameters and the biofilm obtained will be submitted to molecular biology analyses. The project is at the end of Phase 1, with the design obtained and under development of chemically modified electrodes. At the same time, 3 inoculum reactors (INO 1, INO 2 and INO 3) are monitored, which show organic matter removal and Coulomb efficiency. The INO 2 showed 84% of removal and 1.64% of Coulomb efficiency, being the most efficient."

RCGI Project number: 56

Development of BiVO4 particles with exposed facets to boost light-driven CO2 reduction into solar fuels

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Keywords: CO2 reduction, Bismuth Vanadate, Methane

Impact: The serious environmental crisis that humanity is going through and the attempts to recover biodiversity, the economy, life, among others, implement new solutions to face the disasters of global warming. In the context of renewable energy, photocatalysts based on the BiVO4 semiconductor are presented as an interesting proposal, under the mechanism of artificial photosynthesis, which in addition to taking advantage of sunlight as the main natural source, produces products of high added value from CO2, minimizing the impacts of its emissions on the environment.

Highlights: Semiconductor-based CO2 photoconversion and the mechanism of artificial photosynthesis are promising strategies to produce green hydrogen and value-added products such as hydrogen, methanol, ethanol, among others. Studies indicate that BiVO4 has proven to be a promising material for artificial photosynthesis reactions, mainly because it presents a theoretical rate of solar energy absorption of around 9.2% under AM1.5G filter, simulating solar radiation.

Abstract:
The dependence on fossil fuels for energy production, such as oil, natural gas, and coal, results in the emission of large quantities of carbon dioxide (CO2), methane (CH4), and other gases, which are uncontrollably released into the environment. This results in dangerous environmental issues, such as global warming, which affect the lives of millions of people. Given the importance of finding some viable solution to the current environmental crisis, there is an enormous interest in the so-called green energy sources, or renewable energy, that do not generate waste or greenhouse gas emissions. A great source of energy that has been available to us for billions of years: the sun, whose energy source is the most abundant on the planet, and whose use through the application of new technologies has led to the emergence of photocatalysts as an ecologically responsible form of great economic interest. In this context, the conversion of CO2 using photocatalysts suspended in water is an important strategy to explore and produce high value-added products from CO2, minimizing the impacts of its emission. Due to its electronic properties, BiVO4 is a promising material to act as a photocatalyst in the CO2 conversion reaction, however, intrinsic limitations end up limiting its photocatalytic potential. Here, BiVO4 was synthesized by hydrothermal reaction to reach well-shaped particles with exposed facets to boot the conversion of CO2 into CO and CH4. In order to improve the charge separation and boosting the CO2 conversion, p-n heterojunction was formed with BiVO4 and FeNiOx, FeCoOx and FeMnOx. The results indicate that the formation of p-n heterojunction was responsible for the generation of an internal electric field, which drives the photogenerated electrons between the semiconductors, resulting in the suppression of electron – hole recombination, which further photoreduces the CO2 molecule to CH4 and boosting photocatalytic activity of BiVO4.

RCGI Project number: 59

Alcohols Production from CO2 Hydrogenation on Cu-UiO-67 catalysts using H2O as source of hydrogen

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Keywords: CO2 hydrogenation, UiO-67, metal-organic frameworks

Impact: CO2 hydrogenation to higher alcohols is a promising approach, although catalysts with adequate selectivity, activity and stability have not yet been found. In this way, this work aims to explore Cu-based MOFs as catalyst for the CO2 hydrogenation to produce alcohols, mainly ethanol. UiO-67 with distinct copper precursors and different operating conditions will be evaluated.

Highlights:

CO2 hydrogenation to alcohols production, at mild conditions, was performed using Cu-UiO-67 as catalyst.

The impact of different copper precursors as active sites on UiO-67 has been evaluated.

Operational parameters, including the use of H2O as alternative source of hydrogen, have been explored for optimizing ethanol production.

The catalyst UiO-AcCu presented the best productivity to alcohols at 1bar, 3 h, 180 °C and CO2/H2O=3/1.

Abstract:

The use of CO2 has attracted attention in recent years due to the possibility of its transformation into raw material for the production of value-added chemicals. The hydrogenation of CO2 to products of commercial interest, such as alcohols, linked to the use of renewable energy, can curb indiscriminate emissions of this gas and reduce dependence on fossil resources. As this reaction is sensitive to the catalyst structure, the agglomeration of active sites implies a reduction in catalytic activity and selectivity to the product of interest. In this context, MOFs have been investigated due to their potential advantage of generating stable interfaces with these active sites, protecting them from deactivation. In addition, MOFs can control specific sites on the catalyst, making it more efficient for the product of interest, which can be useful to improve higher alcohols synthesis, such as ethanol. With basis on this knowledge, this work aims at the synthesis of Cu-UiO-67 for application in the CO2 hydrogenation. UiO-67, used as support for Cu active sites, was synthesized by solvothermal method for 48 h at 120°C for the formation of crystals. Then, the resulting material was washed with DMF, THF and acetone and dried for 12 h at 60°C. Copper precursors from different salts (AcCu, CuSO4, CuCl2, Cu(NO3)2 and CuI) were incorporated into its structure, via ion exchange, in order to verify the influence on the maintenance of the MOF characteristics and on the productivity of the alcohols in the reaction. The CO2 hydrogenation reaction was carried out at atmospheric pressure, using H2O or H2 as sources of hydrogen. Reaction products were quantified via GC-FID. Using XRD, SEM and FTIR-ATR, it was possible to confirm, respectively, the formation of crystal structures, morphology and characteristic bands of these materials. In addition, by TGA, we evidenced that they were thermally stable up to, at least, 300 °C. From CO2 hydrogenation using H2O, it was possible to verify the formation of alcohols over all the investigated catalysts, mainly on the UiO-AcCu. The most promising ethanol productivity (7.6 µmolEtOH /h.gcu) was obtained at 180 °C, 3 h and H2O/CO2 molar ratio of 3/1.

Synthesis and characterization of heterogeneous catalysts for dimethyl ether production via methanol route.

Miguel Ramon Infante Guerra, Pedro Miguel Vidinha Gomes, Maitê Lippel Gothe

Keywords: zeolite (ZSM-5) , rhenium, dimethyl ether (DME) production

Impact: The methanol to hydrocarbon process (MTH) is a clean an optimal route to produce different and products such as DME. This process could be considered a green replacement for crude oil fuel production. The implementation of this DME production route could lead this technology into an industrial scale, avoiding the utilization of conventional basic synthesis and preventing the thermal energy waste.

Highlights: The methanol to hydrocarbon process (MTH) is a clean an optimal route to produce different and products such as DME. This process could be considered a green replacement for crude oil fuel production. The implementation of this DME production route could lead this technology into an industrial scale, avoiding the utilization of conventional basic synthesis and preventing the thermal energy waste.

Abstract:
"The methanol to hydrocarbon process (MTH) is an optimal route to produce many different and clean products such as DME. This process could be considered a green replacement for crude oil fuel production. The MTH process generally uses a variety of zeolites being the H-ZSM-5 one of the most used. The H-ZSM-5 has great scientific interest and it´s an attractive material because shows a high thermal stability, has many Lowry-Brönsted and Lewis acid sites and could be a support for a series of metals, like rhenium, which could be used to improve the conversion ratios and a better performance.

For that reason, the development of a green DME production route could lead into a gradual implementation of this technology into an industrial scale, avoiding the utilization of conventional basic synthesis and preventing the waste of thermal energy.

In this study, we synthesized a ReOx/ZSM5 catalyst and proceeded to carry out the methanol hydrogenation reaction at 200°C to obtain the DME as our main product. Both catalyst characterization studies (XRD, ICP-OES, SEM) and catalytic studies produced promising results compared to those reported in the literature. A study of the reaction mechanism is also presented here with the aim to improve the catalyst catalytic performance and optimize the reaction conditions. "

RCGI Project number: 63

Development of a Catalytic Process for the Conversion of γ-Butyrolactone Into High Added Value Products Using Supercritical CO2

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Keywords: Biomass, γ-butyrolactone, Supercritical CO2.

Impact: The unsustainability of fossil materials generates the search for alternative production of chemical products from clean and renewable processes. In this context, biomass is considered a source of building-blocks molecules capable of synthesizing high value-added chemicals. γ-Butyrolactone, for example, is an important green source for the production of 1,4-butanediol and tetrahydrofuran, having these products several industrial applications.

Highlights: It was noticed that the effect of temperature and solvent had great importance for the selectivity of reactions. In an essentially aqueous medium, dimers were produced. However, when using a solvent-free medium and supercritical CO2, the reaction path changes completely, resulting in completely conversion to 1,4-butanodiol.

Abstract:
1,4-Butanediol (BDO) and tetrahydrofuran (THF) are a highly valued chemical building-blocks (CBB) used in the production of a widely type of materials, namely polymers, polyesters, polyurethanes, films, fibers, adhesives and plastics. For instance, the incorporation of these products into plastics could improve the biodegradability properties of these materials. However, their production is still based on raw materials obtained from fossil fuels, which raises issues about the sustainability of BDO and THF applications. In this context, it is known that BDO and THF can be produced from the catalytic hydrogenation of γ-butyrolactone (GBL), which can be obtained from different biomass-based products. Nevertheless, the major drawback of this catalytic conversion is related with its selectivity. Therefore, the aim of the present work was to develop a selectivehydrogenation process to transform GBL into BDO and THF using bimetallic catalysts based on rhenium and palladium supported on silica (RePd@SiO2). To accomplish this goal we have studied the influence of the operational parameter temperature and pressure of hydrogen with a central rotational composite design. The impact of scCO2 on the reaction selectivity and the effect of a solvent-free reaction were also evaluated. The results show that only the linear temperature effect was significant for the GBL conversion, while for the BDO selectivity, the quadratic effects of temperature and pressure were statistically significant. Dimers of BDO and GBL were identified as the main products of the reactions and water had a great influence on their formations. In a solvent-free medium, the THF selectivity showed interesting results (93%). Additionally, the results show that the selectivity could be completely reversed by the presence of CO2 showing that scCO2 could be used to tune the reaction selectivity towards a given product. Hence, the increase in CO2 pressure decreased the GBL conversion and completely modified the selectivity of the reaction, reaching 100% for BDO.

RCGI Project number: 63

Solar Energy and Data Science: a prediction model for the Amazon Basin

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Keywords: Solar energy, machine learning, green house gases

Impact: The renewable energies have confirmed their potential to reshape the energy matrix of several countries, in the last two decades, reinforcing the set of actions to better protect the environment. For instance, the solar and wind sources of energy production can dim the production and release of pollutants associated to electricity production. Unfortunately, the atmospheric temperature rise has been linked to the increase of the gas emissions, such as Carbon Dioxide (CO2) and Methane (CH4), from manifold sources, such as the thermal power stations for electricity generation. On the other hand, the pollutants concentration may affect the production of solar energy for instance. This work assess the impact of the greenhouse gases, using machine learning methods, into the capacity to generate the solar energy in the city of Manaus, as a standard case for the Amazon Basin.

Highlights: The Amazon basin has caught special importance for Brazil and abroad, and more recently, data from satellites, fixed instrumented stations and airborne surveys has provided guidelines for studies of the environment impact. One way to reduce the aftermaths of the climate degradation in that region is a broad use of renewable energies, such as the solar option. Due to the weather characteristics of the region, among other factors, the prediction of the solar incidence impacts the economic and social evaluation of this energy option. Thus, the development of machine learning methods to predict the solar incidence (J/m2 per day), considering the greenhouse gases, aids the assessment of this energy generation for the region.

Abstract:
The sun irradiation in Brazil has a non-homogeneous distribution, being measured as W.h/m2 per day. In this work, the data measured came by land stations are the total solar incidence, as a function of the sky cloud coverage, the local temperature (maximum, minimum and mean values), the local atmospheric pressure, the local humidity, and greenhouse gases concentrations and other variables. The satellite can also gather the same data, with a different set of ways of measurement tough. These were the features for the Data Science (DS) methods too. Therefore, the total sun incidence can be set as the output or target variable, and all others variable as the input. As mentioned before, the season can outline another key factor, due to the atmospheric characteristics impacting into the total sun incidence measurement, which varies in time due other physical reasons. The application of DS techniques considered Decision Tree (DT) models and Time Series (TS) as well. For the DT option, the data can be set with the measured total sun irradiance as the target variable, as a function of other variables. Prior to the use of the ML models, a feature importance analysis was carried out. The features linked to the water and pollutants dispersion into the atmosphere explained with more relevance the output. Vector autoregression (VAR), Gradient Boosting (GB), Light Gradient Boosting (LGB), eXtreme Gradient Boosting (XGBoost), Random Forests (RF), and other methods were used with data with a month and week aggregation. The metrics used to evaluate the results were the Mean Absolute Error (MAE) and the Mean Square Error (MSE). The best results of the DT methods came from the LGB and RF. For the TS, the satellite data (as a source) had better results with the use of VAR.

RCGI Project number: 64

CFD Simulation of a fluidized bed reactor using discrete element method in OpenFOAM

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Keywords: chemical looping, discrete element method, fluidized bed reactor

Impact: The simulation of CLC processes following interconnected fluidized bed reactors imposes important challenges. In this work, numerical models of varying levels of complexity are studied in their capacity to predict the operational data and particle dynamics from the air reactor of the 1 MWth CLC pilot plant located at Technische Universität Darmstadt.

Highlights: The pressure drop in the reactor is predicted with the incompressible solver within the same order of magnitude. A methodology for defining the initial conditions of the lagrangian phase is proposed, which has proven to be capable of efficiently predicting the pressure in the reactor. The capacities of three solvers of varying levels of complexity in their numerical models are compared within the purpose of the simulation of CLC reactors.

Abstract:
Chemical Looping is a promising technology for carbon capture and storage (CCS), currently at the early stages of its practical implementation. A typical chemical looping plant is composed of two fluidized bed reactors (air and fuel reactors) interconnect by a particulate metal oxide, so called, Oxygen Carrier (OC), which supplies the required oxygen for the oxidation of the fuel while avoiding direct contact with the air supply. Computational Fluid Dynamics (CFD) simulations play a critical role at capturing the complex physical phenomena within its reactors. In this project, CFD-DEM simulations of the air reactor (AR) of the 1 MWth chemical looping pilot plant located at Technische Universität Darmstadt are performed within the open-source software OpenFOAM. The results of simulations employing three different solvers and models are compared: DPMFoam (for an incompressible laminar flow with four-way coupling and soft-sphere model), CoalChemistryFoam (for a non-reactive compressible laminar flow with four-way coupling and rigid-sphere model) and an in-house solver (by modifying the CoalChemistryFoam to include a soft-sphere model and the Ergun-Wen-Yu drag model for dense particle flows). Furthermore, the effects of parcel modeling on the accuracy and stability of the simulations are briefly studied. Operational data of the plant is used to validate the simulation results and its underlying numerical models. The simulation conducted with the incompressible solver has managed to predict the pressure drop within the air reactor within a short elapsed time. By starting the system with an amount of particles equivalent to the resident mass within the reactor during steady state operation, the pressure drop could be evaluated at a simulation elapsed time (about 1 to 2 seconds) significantly shorter than the required to reach the steady state operation of the reactor (estimated to about 30 to 50 seconds). The parcel modeling has introduced numerical instabilities to the performed simulations, with a highlight to the impacts on the compressible model. Here, the heat transfer rates during initial transient regime were high enough to cause the simulation to collapse. This issue could be mitigated with careful control of the Courant number. Lastly, one of the studied solvers is to be selected for a simulation, in which the operational steady state of the reactor is to be reached.

RCGI Project number: 67

Development of new Deep Eutectic Solvents (DES) for CO2 capture

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Keywords: CO2 capture, carbon dioxide, deep eutectic solvents

Impact: The development of new DES will allow the use of new resources and technologies for the CO2 capture, which will be essential for better efficiency in the capture of greenhouse gas emissions and can lead to new applications as well.

Highlights: This study focuses on the development of new DES (deep eutect solvents), physicochemical characterization of DES/CO2 systems under experimental conditions of the most promising systems for CO2 capture processes

Abstract:
"In the last decades, the concern about global warming has been intensified. Compared to other greenhouse gases, CO2 is the main responsible for the effect. Given the difficulty of replacing current energy sources, the development of methods focused on reducing or controlling emissions has become more relevant. Among the available technologies, the absorption of CO2 with amines is currently the most used in the industry, but its use leads to a large consumption of energy and the use of volatile amines that make the processes more expensive and ecologically degrading.

Among the new technologies developed, IL (ionic liquids), has emerged as a great alternative, given that they have good CO2 solubility, are low volatile and stable in a wide temperature range, they can also be developed with different combinations of cations and anions for specific applications. The main disadvantages are its high viscosity and high production costs, as well as its ability to absorb CO2 in the presence of water. Considered a subclass of ILs that show good performance in CO2 absorption are the DES (Deep Eutectic Solvents), which are composed of a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HDA), forming eutectic systems. It has the advantage over ILs to present similar CO2 absorption capacity, lower toxicity, lower vapor pressure and lower heat of regeneration.

Even with good potential, DES are still not very well characterized and their properties are still being studied. In order to develop new materials for CO2 absorption, in this work we developed a new DES, and determined their chemical and physical characteristics, through techniques such as DSC and NMR, we also studied their CO2 absorption capacity. In order to generate materials with low cost and less environmental impact, we focus on using amino acids and polyols in the mixture of DES, we use HDA and HDB as choline, proline, DBU and conventional polyols. To obtain better interaction with CO2 and decrease hydrophilicity, synthesis of derivatives of the studied HDBs and HDAs were also carried out, focusing mainly on modified polymers or oligomers with functional groups with affinity for CO2.
"

RCGI Project number: 68

What influences public perception of the use of hydrogen as a source of energy?

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Keywords: Public Perception, Hydrogen, Factors

Impact: The positive public acceptance of the adoption of hydrogen-based technologies is an important step towards society's energy transition. In this sense, despite hydrogen being seen as a potential source of explosions, when faced with information on the use of the technology, participants in several surveys started to feel safer with the technology.

Highlights:

- Hydrogen could be one of the important possibilities to stop global warming and limit it to 1.5º in the next two decades.
- Fuel cell electric vehicles (FCEVs) have positive public acceptance rates, which demonstrates their potential for high implementation in the transport market.
- Although people may understand the importance of hydrogen-based technologies, risk perceptions are a major barrier to greater acceptance

Abstract:
In an attempt to mitigate the excess of carbon in the atmosphere, society is faced with the need to adopt alternative sources of energy. The use of hydrogen, even though it has long been known as an energy source, in recent years has come to be considered an efficient option for decarbonizing the economy due to the potential of reducing emissions and being a substitute for fossil fuels. With this new paradigm in mind, it is necessary to seek an understanding of how society will react to the broad use of this new source of energy, as well as its implementation and management impacts. In this way, this study intends to understand and assess which factors are responsible for modulating public opinion regarding the use of hydrogen as a sustainable energy source. A literature review was carried out to analyse 32 articles about social perception regarding the use of hydrogen retrieved from Scopus. According to the main findings, both public awareness and people's knowledge about the possibilities of using

RCGI Project number: 70

STATE OF THE ART OF THE SOCIAL PERCEPTION OF RENEWABLE ENERGIES - WIND AND SOLAR

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Keywords: social perception, renewable energy, wind and solar

Impact: Renewable energy tends to be highly accepted by the general public as a clean energy source. However, perceived resistance arises in the local community against renewable project installation, through the well-known NIMBY effect. Understanding social perception and acceptance of renewables is key to growing the potential deployment of clean energy.

Highlights:
- The high acceptance as clean energy sources of both renewable energies.
- The presence of NIMBY (Not In My Back Yard) effect is related to the local resistance of renewables installation in the vicinities
- Brazil has a high potential to install renewable energy which will require further investigation into renewables social perception and acceptance.

Abstract:
This panel exposes the state of the art of the social perception of renewable energies (wind and solar) in Brazil and other countries. Wind energy stems from the conversion of kinetic energy from the movement of winds and solar energy from the conversion of solar radiation into energy (direct and indirect). The major social perception feature of both energies is their general high acceptance as clean energy sources. That high acceptance is mediated by a reaction known as NIMBY (Not In My Back Yard) effect in the local arena when society tends to refuse renewables installation in their region. Among the most considered factors that impact public perception and acceptance of these renewables are the expected costs and benefits, social, economic and environmental risks, trust and perceived fairness. Furthermore, the perception of wind is influenced by the visual impact and noise annoyance, just as the perception of solar is influenced by the belief of its low benefits. Thus, understanding social perception and acceptance of renewables in the Brazilian context is key since the country has a high potential to install renewable energy, as it exhibits a wind volume twice the world's average and a high incidence of sun all over the territory all year long. In the political context, renewable energy presents a key role in energy diversification. Despite its role, this kind of energy has slow growth in Brazil and very few studies on renewables' social perception.

RCGI Project number: 70

First principles studies of ZIF-67: structural transitions on mesoporous materials for membrane technologies

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Keywords: DFT calculations, ZIF-67, nanofiltration membrane

Impact: The produced water from O&G exploration contains metals and pollutants, such as Boron and Lithium. This research studied the ZIF-67 structure, which can be used as a nanofiltration membrane to separate the ions from PW. By applying hydrostatic pressure to the ZIF-67 structure, we observed a structural phase transition, with no significant changes on the electronic structure, which may not influence the filtering characteristics of the material.

Highlights: DFT calculations show that there is a hydrostatic pressure structural phase transition of the ZIF-67.
The findings obtained in this work may guide to design and manufacture nanostructured materials for the separation of Li and B from PW.

Abstract:
"The produced water (PW) from O&G exploration contains large amounts of metals and pollutants, such as Boron (B) and Lithium (Li) [Ezechi et al., 2012]. There are social and economic interests, and technological challenges in developing methods for treating PW as a source of human and agricultural consumption [Igunnu & Chen, 2014]. The PW treatment can be done by various methods including physical methods such as membrane filtration. 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 the transport and thermodynamics properties of a subclass of MOFs, the Zeolitic imidazolate structure (ZIF). ZIF systems exhibits mechanical flexibility, and has received extensive research interest in this subject area [Zhong et al., 2018]. In particular, we focus on the ZIF-67 structure, which can be synthesized by a facile and environmentally friendly organic synthesis method and has characteristics of a tunable pore aperture, which is ideal for filtration processes. We employ Density Functional Theory (DFT) using the plane-wave basis projector augmented wave method and optB86b-vdW [Klimes et al., 2011] exchange-correlation functional as implemented in the VASP package. By applying hydrostatic pressure to the ZIF-67 structure, we observed a structural phase transition for a lower energy structure with angular structural variations of the organic ligands. We fitted the total energy with respect to the volume using the Rose-Vinet and the Birch-Murnaghan equations of state for both phases. The equilibrium volume and the bulk modulus for each one were determined. No significant changes on the electronic structure have been observed, which indicates that the structural change may not influence the filtering characteristics of the material. The findings obtained through DFT and MD may serve as an essential guideline to design and manufacture nanostructured materials with unique properties for the separation of Li and B from PW.
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RCGI Project number: 72

Integer linear programming applied to inversion problems in time domain acoustic wave propagation

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Keywords: Acoustic Inverse Problem, Integer Linear Programming, Time Domain

Impact: Acoustic inverse problems with sharp interfaces are challenging since interface misidentification leads to large timing and wavepath estimation errors. We propose incorporating the sharp interface hypothesis into the model through a discrete control variable, thus avoiding the appearance of regions with smooth transitions, and defining the position of interfaces with no ambiguity,

Highlights:
* Discrete control variable that unambiguously defines sharp interfaces.
* Application to Acoustic Inverse Problems of tools from Topology Optimization and from the Adam optimization algorithm to sensitivity filtering.
* The parameter field is allowed to change its topology along the inversion process: Initial guess and final result can have a different number of inclusions.

Abstract:
"The acoustic inverse problem in the time domain featuring wave velocity model reconstruction with sharp interfaces is addressed using an integer control variable approach.
The inversion procedure aims at finding the parameter field that minimizes a least-squares misfit function with respect to data generated from a synthetic model.
The wave equation is modeled using the Finite Element Method.
The proposed optimization methodology is based on a sequential Integer Linear Programming formulation used in the field of Topology Optimization.
Since this is a gradient-based technique, the sensitivity with respect to the integer control variable is evaluated by the adjoint method. Sensitivities are modified using both damping filters and Helmholtz-type filters to deal with the ill-posedness that is inherent to this class of inverse problems.
The integer control variable naturally incorporates the sharp interface hypothesis,
whereas a continuous control may generate transition regions with intermediate values
and no clearly defined boundary.
The damping filter is successful in controlling instabilities by incorporating the whole optimization history to the control update.
Furthermore, the generality and effectiveness of the proposed framework is evaluated by addressing both 2D and 3D problems with sharp interfaces taken from the literature.
"

RCGI Project number: 46

Lanthanum strontium-doped manganite modified with nickel for SOFC applications

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Keywords: Solid oxide fuel cell, perovskites, LSM modified with Nickel.

Impact: The solid oxide fuel cell (SOFC) is an electrochemical device that can operate with very high energy conversion efficiency. With the discovery of new materials and designs, currently, SOFCs operate at s temperature nrsr to 600º C, allowing the direct use of flexible fuels such as ethanol. One improved approach has been the use of Ni-modified perovskites in the anode, as those used in this work.

Highlights:
Intermediates temperatures SOFC operation
Ethanol as SOFC fuel
Perovskites modified with Ni
Better SOFC operating conditions
Increased SOFC cell life

Abstract:
"The solid oxide fuel cell (SOFC) is an electrochemical device that can operate with very high energy conversion efficiency, at temperatures between 600°C to 1000°C. Several studies are being conducted to improve the SOFC design to allow the use of fuels arising from renewable sources, such as ethanol. Also, research with different electrocatalytic materials has been focused on reducing the operating temperature to broad the range of applications and/or reducing the operating temperature.(1, 2)
In this work, a SOFC anode/electrolyte layer was prepared by using a lanthanum strontium-doped manganite (LSM) perovskite modified with 5 wt.% of Ni (here called LSMN) and submitted to a heat treatment at 1100°C for 2 h. This catalytic material was then mixed in a ball milling with 30 wt.% of an electrolyte composed of cerium oxide doped with gadolinium, Ce0,9Gd 0,1O2-δ-CGO, so to form the anode/electrolyte composite layer. This system was then characterized by X-ray diffraction and scanning electron microscopy and finally incorporated to a SOFC half-cell containing an air breading cathode formed with the LSM catalyst and scandia stabilized with zirconia (ScSZ) as electrolyte.
The electrochemical performance evaluations of such SOFC system were conducted by electrochemical impedance spectroscopy and polarization measurements at 700 and 800º C, using 96% ethanol or pure H2 as fuels. Stability studies were conducted by chronoamperometry recorded at the cell potential of 600 mV. Results with the ethanol fuel indicated an overall ohmic cell resistance of 0.4 Ω and a better performance of SOFC at 800 oC, that remained approximately constant for over 20 h. The LSMN perovskite presented a relatively better electrocatalytic activity when H2 was used as fuel, in which case the current density at 600 mV resulted above 220 mA.
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RCGI Project number: 57

Effects of CO2 dissolution in electrochemically-relevant Ionic Liquids

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Keywords: Ionic Liquids, CO2, absorption

Impact: CO2 capture and storage has usually been done with organic solvents that are harmful and not recyclable. Ionic Liquids, which first emerged as alternative solvents, present reasonable capacity to absorb CO2, along with proven electrochemical properties that possibly allow the reduction reaction to occur in their environment. Computer-simulated IL systems provide insights into the mechanisms of CO2 dissolution and point to the best combination of cations and anions for the reduction reaction.

Highlights: Several electrochemically-proven ions were shown to have considerable affinity for carbon dioxide under simulation conditions, which included ambient pressure and temperature. Their viscosities did not change appreciably during absorption, but just enough to facilitate the CO2 reduction reaction even in bulkier of the systems.

Abstract:
"With the growing need to control the amount of CO2 in the atmosphere to mitigate global warming, research on carbon capture and storage (CCS) has gained prominence around the world. Besides being removed from the atmosphere, captured carbon can be made into products with high added value, but the conversion processes are yet to be developed. Current CO2 capture technologies frequently use harmful amine solvents in liquid phase that are volatile and corrosive, thus needing to be replenished and impacting the capture system's long-term reusability. Ionic Liquids (ILs) are promising alternatives for carbon capture and transformation due to their considerable economic advantages: they can be recycled many times and used at standard laboratory conditions, reducing the need for energy input. It is generally believed that ILs are also environmentally friendly, as they are seen as solvents for the emerging green chemistry. Because of their ionic nature, ILs are good electrolytes and have largely been used in the search for novel battery and capacitor technologies. Consequently, they possibly make for a good reaction environment for the electrochemical reduction of CO2. There is, however, a large number of possible ion pairs that can be made into ILs and it would be wasteful to synthesize and characterize all them. Thus, computational models were chosen to evaluate the effects that CO2 absorption can have on the physicochemical properties of electrochemically-relevant ionic liquids, such as phosphonium salts.
In this research, phosphonium cations were combined with three different anions known to have feasible electrochemical windows for the reduction reaction. Extensive Molecular Dynamics simulations were then utilized to calculate the theoretical values of the system's transport properties. It is important to understand the liquid's capacity of absorbing carbon dioxide whilst still keeping solubility and viscosity properties that allow the reaction to take place, as these properties are usually inverse-related. The best candidates for CO2RR environment will then be assessed experimentally to verify theoretical predictions against real-world use."

RCGI Project number: 60

CO2 hydrogenation to higher alcohols catalyzed by ReOx/MgO

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Keywords: CO2, ethanol, catalysis

Impact: ReOx/MgO was able to catalyze the hydrogenation of CO2 to higher alcohols under supercritical conditions

Highlights: A catalyst based on rhenium and magnesium oxide was synthesized and characterized. ReOx/MgO was able to catalyze the hydrogenation of CO2 to alcohols, including higher alcohols such as ethanol, propanol and butanol.

Abstract:
"Nowadays, much has been discussed about the possible damages caused to the environment and to humans about the intense emission of residues from the burning of carbon in the atmosphere. One of the possible solutions to the problem is the active removal of carbon from reactions catalyzed by certain materials, with CO2 capture being the main focus. For this, a study was carried out with the catalysis using rhenium on magnesium oxide for the production of superior alcohols. Rhenium was chosen as active methanol since it has been shown to be active on the hydrogenation of CO2 to methanol, and MgO, a basic oxide, was included with the aim of shifting the selectivity to higher alcohols.
The CO2 catalysis involving rhenium supported on magnesium oxide presents as major conversion products CH4 (methane gas) and carbon monoxide, but it is also possible to notice the formation of a considerable amount of methanol and propanol, under favorable temperature conditions. The method used was the batch method, in which the reactions were carried out at 250 and 200 degrees Celsius, with 75 bar of hydrogen and 25 bar of CO2. The catalyst used was ReOx/MgO synthesized by the wet impregnation of Re2O7 on MgO.
The reactions were analysed by GC-TCD for gaseous products and GC-FID for liquid products. Gaseous products obtained were CO, CH4 and C2H6, and liquid products were methanol, ethanol, propanol and butanol. The reaction temperature was varied in order to evaluate its influence on selectivity. Finally, a greater improvement of the techniques used for the best selectivity of the reaction is sought, aiming at increasing the CO2 conversion to ethanol from changes in the catalyst synthesis and reaction conditions. With this, there will be greater progress in research and environmental preservation."

RCGI Project number: 63

The acetic acid synthesis from ethanol and water: The role of Al in the Cu, Zn, Al-based catalyst.

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Keywords: acetic acid, ethanol, water

Impact: Acetic acid can be generated by the selective oxidation of ethanol. However, to avoid ethanol combustion, this biofuel should be employed at a low concentration in air (4.3%), causing constraints from the economic point of view. Thus, the use of water as oxidant agent is welcome in order to make feasible the generation of this commodity from a renewable feedstock.

Highlights: The acetic acid selectivity is correlated with the acid properties of the catalyst.
Increasing the Al content increases the acetic acid selectivity.
The presence of the CuZn alloy is crucial to acetic acid formation.

Abstract:
Previous studies of our group, shown that Cu, Zn and Al-based catalysts are promising for the generation of acetic acid from ethanol and water. However, these solids show relatively low selectivities (~ 50%) of acetic acid and moderate activity. In order to generate information that guides the proposal of new catalysts and also the improvement of known systems, it is intended to define the role of each component of the catalyst employed in the acetic acid synthesis. In this context, the starting point was a catalyst prepared via Cu and Zn-based co-precipitation (atomic ratio Cu/Zn = 1), which the only precursor (specie identified before calcination) is the aurichalcite ((Cu, Zn)5(CO3)2(OH)6). This compound promotes a strong interaction between Cu and Zn. After reduction two compounds were identified: the CuZn alloy and nanoparticles of ZnO doped with Cu. This catalyst is very selective to acetaldehyde and slightly selective to acetic acid, having almost no acidity evidenced by NH3-TPD. Thus, different Al contents (3, 6, 10% wt. of Al2O3) were added to the mentioned catalyst. Increased Al content, from 6%, leads to a significant increase in selectivity to acetic acid and decrease to acetaldehyde. The addition of Al also causes an increase in the acidity of the catalysts observed by NH3-TPD. Replacing Al with Ga or In in this system, it was found that Ga show a behavior similar to Al. On the other hand, the In-containing catalyst exhibits very low acidity, resulting in low activity. The proposal is that the presence of Al would promote the adsorption of acetaldehyde, avoiding desorption and facilitating its oxidation, i.e., the formation of acetic acid. The Cu content of these catalysts was also modified (half the amount of CuZnAl-6 at% catalyst was used). There was a very significant drop in acetic acid selectivity, an increase in acetone formation whereas the activity do not change. It may be suggested that the desorption of acetate species as acetic acid occurs when this species are adsorbed on the metal/alloy. When the system has less metal on the surface there would be a greater tendency to condensation of acetates and acetone formation. In this context, is being studied the optimization of the catalyst composition.

RCGI Project number: 63

Catalytic conversion of short-chain alcohols using CO2 as auxiliary gas

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Keywords: MTO, ETO, CO2

Impact: Dependence on fossil reserve increase to their depletion has led to another problem in the 21st century: the high concentration of carbon dioxide (CO2) in the atmosphere. To mitigate a large amount of gas released into the environment importants strategic lines are advanced for CO2: capture, storage, and utilization. However, a different method of using CO2 can be raised. Application of carbon dioxide in the context of MTO and ETO reactions.

Highlights:

The use of CO2 as auxiliary gas causes an increase in the maximum yield of light olefins in addition to causing an increase in catalyst uptime.

Abstract:

Currently, ethylene and propylene are the most produced raw materials in the petrochemical industry, obtained principally through well-established cracking processes. The high interest in these light olefins is due to their extensive application as building blocks. Therefore, the most promising solution is the catalytic conversion of short-chain alcohols (such as methanol and ethanol). The catalytic performance of methanol to olefins (MTO) and ethanol to olefins (ETO) reactions depends on forming organic intermediates confined in the pores of the zeolite structure. The appearance of these intermediates is part of the mechanism known as the hydrocarbon pool (HCP). An induction period of just a few minutes is required to generate HCPs formed by aromatic compounds of different sizes that suffer alkylation with methanol or ethanol and subsequent cracking process to form light olefins. Unfortunately, HCPs can also rapidly evolve into higher polycyclic aromatic hydrocarbons (PAHs), leading to catalyst deactivation, obstruction pores, and consequent loss of catalytic activity. The advances in this science area are related to changes in the catalyst structure, studies on the variation of reaction conditions, and the addition of water vapor to the system. However, very little has been observed in these studies regarding the nature of the carrier gas. Therefore, this work proposes using CO2 as a carrier gas in the MTO and ETO processes, ensuring greater reaction efficiency and suggesting a new route for its use, since it is one of the main constituents of the gases responsible for the greenhouse effect. We carried out experiments of methanol/ethanol reactions in CHA and ZSM-5 zeolites with CO2 under the same conditions already well established in the literature to monitor the effects caused in terms of catalyst activity over time, as well as the selectivity of the material. The results show conversion profiles and selectivity tend to vary with the reaction time, whether in the presence of N2 or CO2. However, the change causes an increase in the maximum yield for light olefins, in addition to extending the catalyst activity. Thermogravimetry reveals that CO2 causes a lower temperature variation of the components associated with polyaromatic compounds. The change in these components suggests that the polyaromatic HCP compounds underwent significant changes, thus ensuring catalyst survival and increasing maximum olefin yield.

RCGI Project number: 63

Neural network model for classification of net CO2 fluxes scenarios in the Tapajós Forest, Amazon.

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Keywords: Carbon budget, Net Ecosystem Exchange, Machine Learning

Impact: Neural network classification model is able to predict carbon source, sink and neutral conditions in the Tapajos Forest in Amazonia, based on environmental variables. Carbon sink conditions are favored by increased solar radiation and latent heat fluxes. Neural networks is a promising technique to upscale local carbon budget conditions based on surface and remote sensed environmental variables in Amazonia.

Highlights:

- Neural network classification model is able to predict carbon source, sink and neutral conditions in Amazonia
- Carbon sink conditions are favored by increased solar radiation and latent heat fluxes

Abstract:
The Amazon rainforest has a great influence on the global energy balance and carbon fluxes, responsible for the net removal of approximately 4 million tons of carbon per year, via photosynthetic activity. Climate change and deforestation have impacts on the carbon budget in Amazonia, transforming CO2 sink areas into sources. Given the complexity of the factors that govern the carbon exchange in the Amazon and its influence on biological processes, the use of Data science strategies can promote a better understanding about the main environmental factors for different scenarios, and also, assist in public policies to mitigate the global warming effects. This study aims to identify the environmental factors that determine the temporal variability of carbon exchanges between the biosphere and the atmosphere in the Tapajós National Forest, in the Amazon. Data Science strategies were applied to in an integrated dataset of ground-based carbon flux measurements and remote sensing data, considering the period between 2002 and 2006. An artificial neural network (ANN) classification model was developed to identify the environmental variables with great impact on carbon source, sink and neutrality conditions. The average global score of ANN model was 65%. It was possible to identify the predictor variables with greatest impact to the carbon sink condition: radiation at the top of the atmosphere, sensible and latent energy fluxes and leaf area index. Thus, the ANN model with an ensemble of Data Science strategies can improve a better understanding of variability CO2 fluxes and be a powerful tool to promote new knowledge.

RCGI Project number: 64

Technical and economical feasibility study of the use of Brazilian biomass in chemical looping combustion.

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Keywords: BECCS, chemical looping, computer simulation.

Impact: A study of the technical and economical feasibility of the usage of Brazilian biomass in CLC was successfully conducted. An additional outcome of this study is a computational tool for the dimensioning of a CLC steam cycle.

Highlights: From the assessment of different types of biomass, sugar-cane bagasse has been demonstrated the most promising choice. Specific features of CLC and a steam cycle have been included in a computational code for reactor dimensioning. From the economical analysis, CLC fueled with sugar-cane bagasse has been demonstrated a feasible and competitive choice among existing power plant configurations.

Abstract:
The chemical looping combustion (CLC) is a promising technology, which allows the usage of biomass as a fuel for power generation and CO2 capture. The CLC cycle may consist of two reactors: the fuel reactor and the air reactor. In the fuel reactor, biomass is burned using metal oxides, which are oxidized in the air reactor. As a result, a nitrogen-free flow is obtained, which considerably reduces the energy costs involved in carbon dioxide separation compared to other carbon capture processes. With this in mind, the study aims to (1) identify opportunities for the use of Brazilian biomass in the CLC cycle, (2) determine the average configuration of a plant operating with this technology, and (3) determine the main costs involved in installation and operation through computer simulations. At the end estimated costs are compared with models of current plants and thus determine the economic viability of the plant. To determine the most suitable biomass sources for use in CLC reactors, a bibliographic survey of agricultural production reports is carried out, as well as an analysis of the composition of agricultural waste. From these data, the average production of the different residues and their distribution in the Brazilian territory was determined. With the result of this study, it is possible to estimate the average size of the thermoelectric plant. From this value, a plant configuration is defined and a heat production target is established for the air reactor, which will serve as a steam generator for a power cycle. Bearing in mind that CLC is still not a mature technology, the reactors are dimensioned to determine their characteristics as well as those of auxiliary equipment. The design is performed using the free software Octave. The air and fuel fluidized bed reactors are modeled in the PFR and CSTR cases, respectively, operating with Cu/CuO as oxygen-carrier particles (OC). From this simulation, the air and fuel inputs are established. By solving differential equations linked to the reaction rate in the reactors, the volumes of the fuel and air reactors are calculated. Finally, the operation of the entire plant is simulated and its main components are specified in order to estimate the main costs involved in construction and operation. The resulting values are compared with existing data of power plant configurations.

RCGI Project number: 67

Functionalized hyperbranched polyglycerols for applications in the capture of CO2 and catalysis.

Gabriel Silveira dos Santos, Reinaldo Camino Bazito.

Keywords: Hyperbranched polyglycerols, deep eutectic solvents, CO2 absorption.

Impact: New materials and technologies should be studied to mitigate and reduce greenhouse gas emissions. Deep eutetetic fluids present themselves as a viable alternative to this work due to their intrinsic characteristics.

Highlights: New materials were synthesized for CO2 absorption. Mixtures of choline chloride hyperbranched polyglycerols and superbase modified hyperbranched polyglycerols were synthesized and characterized for CO2 absorption studies.

Abstract:
"The process of capturing anthropogenic atmospheric carbon dioxide (CO2) for
storage or its transformation into other value-added products have attracted increasing attention from the scientific community due to the patent concern of global warming intensified by high greenhouse gas emissions. Research for CO2-absorbing materials, such as deep eutectic solvents (DES) has grown increasingly since their characteristics are advantageous when compared to other liquids, such as ionic liquids and ethanolamine solutions and their derivatives.
DES are liquid mixtures derived from two or more molecules that interact with each other by hydrogen bonds resulting in an intense lowering at the melting point of the product. They have negligible vapor pressure and are very versatile as application because they can be synthesized from several different substances, similar to ionic liquids, however, starting from lower cost materials and, in general, less toxic.
The purpose of this project is the development of deep eutetic solvents for CO2 absorption at ambient pressure and high pressures at different temperatures and to evaluate the selectivity of absorption in gas mixtures.
The synthesized materials are composed of hyperabranched polyglycerols (HPGOH) of low molar mass, acting as a hydrogen bridge donor, and an organic salt as hydrogen bonding acceptor, for example choline chloride (ChCl). The HPGOH were synthesized by the cationic ring opening polymerization of glycidol with 1,1,1-tris(hydroxymethyl)propane (TMP) as the polymer nucleus. The polymers were characterized by carbon and hydrogen NMR spectrum, mass spectrometry (MALDI-TOF) and differential scanning calorimetry (DSC). Mixtures of PGOH and ChCl were made by varying the amount of ChCl to evaluate the impact on the melting point of the product. Attempts were also made to modify the polymer with 1.4-diazabicycle[2.2.2]octane (DABCO), a superbase, to potentiate the interaction of the polymer or the mixture with CO2.
As future perspectives, the mixtures of PGOH, functionalized or not, with other substances, will be synthesized and characterized by Hydrogen and Carbon NMR, mass spectrum and DSC. Studies to determine the absorption capacity and selectivity for CO 2 will also be carried out."

RCGI Project number: 68

Understanding the Public Perception in CCS literature

Guilherme Porfirio Baccari (IPUSP), Karen Louise Mascarenhas (RCGI), prof. Sigmar Malvezzi (IPUSP)

Keywords: Public Perception, Carbon capture and storages (CCS), Social Psychology,

Impact: The assessment of the aspects that module public perception and acceptance of CCS is fundamental to be considered when planning the deployment of future projects and capital investment. Therefore, this work provides an overview of how the concept of "Perception" and "Public Perception" is used and understood in CCS literature.

Highlights: Through 181 articles raised from Scopus database we assessed the main aspects that module public perception and acceptance of CCS technology as well as the subjacent psychological processes. We found Wüstenhagen or Huijts to be the major conceptual axis in the field, even though the majority of articles didn't present a clear definition of 'perception', 'public perception' or 'acceptance'.

Abstract:
Carbon Capture and Utilisation and/or Storage (CCU, CCUS or CCS) is a promising technology that intends to mitigate greenhouse gas (GHG), and especially CO2, emissions worldwide towards net-zero, following the Paris Agreement. However, CCS projects are usually big infrastructure initiatives that demand high initial investment as well as suitable storage sites. Previous experience has demonstrated that stakeholders' compliance and public acceptance are key elements for successful implementation, otherwise, such projects may be cancelled midway through, such as in the infamous Barendrecht facility, resulting in investment loss. Such aspect of the CCS implementation, also known as public or social perception, is often overlooked in research or treated superficially and, therefore, we intended to fill this gap. Our team raised 218 articles through the Scopus database regarding 'public perception/ acceptance' or 'social perception/ acceptance', and 'CCS', from which manual analysis revealed 181 related to the theme and only two to Brazil. Using a qualitative and quantitative mixed-method and a grounded theory methodology, we found out that, notwithstanding Wüstenhagen or Huijts concept of social acceptance were preeminent, most of the articles hadn't a solid theoretical framework on which to base their studies. Many of the researchers came from an engineering and technical background and were not used to the concepts developed in the social sciences, and social psychology, to deal with an in-depth understanding of individual and social phenomena, such as public perception. Based on those findings we analysed what were the understanding of Public Perception and Acceptance present on those articles and the underlying assumptions in their so-called theories and methodologies, typically the survey. Results showed that many factors play a role in CCS acceptance, such as people awareness, knowledge, trust, susceptibility to the NIMBY (Not In My Back Yard) effect, benefits and risks perception, socio-demographic factors, willingness to pay for the technology, acceptance and preferences between technologies, Governmental Policy and interactions among stakeholders. Also, analysis found those factors are modulated by context and sub-factors which may or may not be present in every category. Future investigation should aim for field research and interventions within those categories, and also the theoretical consolidation of the area of study.

RCGI Project number: 70

Citizen Science Approach to the Creation of a Molecularium

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Keywords: Citizen Science, Molecular Dynamics, Virtual Reality

Impact: With the rise of virtual spaces and quasi-instantaneous information, wicked problems like the uncertainty of risk, science mistrust, and misinformation are exposed. In this scenario, there is room for science dissemination tools in those spaces. Here, we propose the creation of a Molecularium, which uses similar technologies to engage the public in molecular science based on databases fed by a citizen science program.

Highlights:
Experimentation of Molecular Dynamics with the Molecularium, a virtual reality platform that uses sensorial experience.
Citizen science as a bridge to public engagement and active science production, leading to a database of interactions and creations by the public.
Dissemination of the Molecularium via augmented reality to promote a larger database based on public perception

Abstract:
"The Molecularium is a virtual educational platform loosely inspired by the planetarium, but instead of focusing on the planetary and galactic scale, it will focus on the molecular scale. This platform allows new immersive experiences on visualization and interaction with molecular systems. The main idea of the interactions is to teach the concept of molecular dynamics through sensorial experiences, in a meta approach, to feel the impact of the molecular dynamics in a diverse scenario. In particular, their impact on the macroscale, such as environmental issues. All the interactions will be saved as original creations by the public and a database will be created. The RCG2I database will provide the structures for the interactions. The strategy for user-based experience is to use virtual reality because immersion can increase public engagement. Also, the quick rise of virtual reality technologies offers tools that increase the realistic feeling of the interactions, such as special suits, gloves and trackers. The augmented reality approach is also possible since the requirements of running this technology are available with modern phones. Then, one can see the molecular structures in everyday environments, which can be used as a form to describe the unseen phenomena of those environments.
The main sensorial response will be the sound based on different interactions over the molecules. The molecule manipulation can trigger a sound synthesis, which represents this interaction. The sound is produced by a modular synthesis, where the interaction data is applied to simulate the system's molecular dynamics. A set of parameters can be explored to control the synth parameters, such as pitch, volume and panning, while the simulations run in real-time during the immersion experience. The Molecularium will be running in the Unreal Engine, a game engine optimized for Virtual Reality, which allows real-time calculations and sound synthesis. The public interactions are the focus, not only for science communication, but also for building active contributions in the database, public perception and decision-making provoked by the molecular dynamics experience. The sound creations bring the public in an authorship position, and the immersion may close the gap in the scientific production and appropriation of means of knowledge.
"

RCGI Project number: 70

Separation of Li+/Na+ ions by using nanoestructured materials, polarization and DFT calculations

Rafael dos Santos Domingues, Caetano Rodrigues Miranda

Keywords: Selectivy, membrane, DFT.

Impact: This work intends to identify molecular mechanisms that act on the selectivity of ions and use this acquired knowledge to develop a new way to acquire Li+ by separating it from other ions, especially from Na+, on produced water, by using graphene oxide membrane and DFT calculations, to help supply the growing demand for Li+.

Highlights:
Identification of molecular mechanisms on the Li+/Na+ selectivity.
Utilization of graphene oxide base membrane on separation of Li+/Na+.
Polarization effects of functional groups on Li+/Na+.

Abstract:
The demand for lithium compounds is increasing in the world, especially for the use of lithium-ion batteries. However, Li production is bound to surpass by its demand in a near future. Furthermore, its extraction from natural resources is challenging due to the extreme semblance of the Li+ and the Na+, and the toxicity to the environment. One potential source of Li is the produced water from the O&G exploration. In this work, we aim to understand the underling molecular mechanisms to separate selectively monovalent ions from produced water. One possible strategy is to use nanostructured materials to polarize cations to form a covalent character in a predominantly ionic bond. To access the electronic properties and select the best materials, first principles calculations based on the Density Functional Theory are performed to determine the ionic energy of adsorption and electronic structure modification. In particular, we will focus on the oxide graphene based compounds for membrane technologies, the role of Oxygen based functionals groups and study polarization capacity of Li+/Na+ ions.

RCGI Project number: 72

simwave - A Finite Difference Simulator for Acoustic Waves Propagation

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Keywords: Acoustic wave propagation, Finite differences method, High performance computing.

Impact: simwave implements the kernel of applications such as the full-waveform inversion (FWI), and the reverse-time migration (RTM). Its Python front-end enables straightforward integration with many existing Python scientific libraries for the composition of more complex workflows and applications (e.g., FWI, RTM). Its development has been motivated to support the research in seismic inversion methods and in high-performance computing (HPC).

Highlights: simwave is an open-source Python package to perform wave simulations in 2D/3D domains. It solves the constant and variable density acoustic wave equation with the finite difference method and supports domain truncation techniques, several boundary conditions, and the modeling of sources and receivers in a user-defined acquisition geometry. Its back-end implemented in C enables performance portability across a range of computing hardware including CPUs and GPUs.

Abstract:
"Acoustic waves are a means of energy propagation through a medium in space. These waves travel with a characteristic velocity and exhibit phenomena like diffraction, reflection and interference as they interact with the medium. The propagation of acoustic waves can be described by pressure variation, particle velocity, particle displacement, and/or acoustic intensity.

The propagation of acoustic waves is often used as a remote sensing tool to probe domains that are otherwise difficult to physically observe. Depending on the properties of the medium and the application, the simulation of acoustic waves may or may not consider variations in material density. For example, the acoustic wave equation with a constant density approximation is frequently used in seismic inversion workflows to estimate the P-wave velocity in the ground, which is later used to help locate raw material deposits such as oil and gas. In medical imaging, similar methods are used that consider variations in material density or elasticity to study and diagnose tumors and other lesions in the human body. Acoustic tomography also plays an important role in understanding and monitoring ocean processes such as the global tides and internal waves and atmospheric turbulence. In structural modeling, the acoustic wave can be used to identify failures in complex structures such as bridges and buildings.

Many wave propagators are part of comprehensive propriety codes that are developed by companies for industrial-grade workflows. In this context, usually, the software is not available to independent researchers. Often many of these industrial workflows require computationally efficient implementations that can be used at many different computing scales, and this implies that re-implementation at some level is required.

simwave is a Python package that enables researchers to model acoustic waves propagation using short Python scripts with implementations that are verified and optimized for high performance. To be useful

to a wide range of applications, the package is made to be flexible across hardware and software environments. Users interact with simwave with a Python application programming interface (API) by passing user inputs that control the desired accuracy of the simulation. Many components of simwave are implemented for applications with geophysical exploration and the simulation of waves can occur with either the assumption of constant or a variable density medium."

RCGI Project number: 46

Microkinetic Modeling of Ethanol Electro-oxidation Reaction

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Keywords: microkinetics, ethanol, electro-oxidation

Impact: Microkinetic modeling helps to understand the complex dynamics between different intermediates produced in ethanol electro-oxidation reaction and could lead to the discovery of better catalysts.

Highlights: A detailed reaction scheme for ethanol electro-oxidation is proposed based on literature review. A set of Ordinary Differential Equations describes the temporal variation of adsorbed intermediates. Electrochemical experiments can be simulated with special enphasis for the response in the oscillatory regime that can be seen as a 'fingerprint' for the reaction.

Abstract:
The oxidation of molecules derived from biomass has been used both directly in fuel cells and for the production of clean hydrogen. These processes represent an important alternative for replacing internal combustion engines based on fossil fuels. Despite decades of studies, the interconversion of chemical energy into electrical energy (an object of electrochemistry, and particularly of electrocatalysis) still presents challenges. The electro-oxidation of small organic molecules (up to six carbons, for example) is one of the possibilities studied, with ethanol among them, however, practical applications still found technical and economical limitations. Combining experimental and theoretical knowledge to model these complex reactions can help in understanding the kinetics and in the rational development of new catalysts. The objective of this research project is to apply microkinetic analysis to develop models that describe different phenomena observed experimentally in the electrocatalytic oxidation of ethanol under different reaction conditions. A microkinetic analysis describes the temporal variation of intermediate species adsorbed onto the surface of a catalyst throughout a reaction. The knowledge of the degree of coverage for each species then allows the simulation of techniques used in electrochemistry. Here we will present the reaction scheme proposed for ethanol electro-oxidation, the mathematical model that describes it and some experimental data that will be simulated.

RCGI Project number: 57

Study of CO2 plasmon-assisted electroreduction over Cu2O-Au nanostructures towards C2 compounds synthesis

Leonardo Domenico De Angelis, Susana Inés Córdoba de Torresi

Keywords: Electrocatalysis, CO2, Plasmonics

Impact: The use of fossil fuels has led to undesired environmental changes, such as global warming, acidification of oceans and rainwater, among other issues. The further consumption of these energy sources and lack of regard for the anthropogenic production of CO2 could led to irreversible consequences. This project aims at utilizing plasmon-assisted electrocatalysis with controlled electrocatalyst morphology to convert CO2 into value-added C1 and C2 chemicals.

Highlights: By fine-tuning Cu2O electrocatalysts in nanometric scale, we were able to convert CO2 into gaseous products such as CO, CH4 and C2H4. Furthermore, it was possible to control which reactions pathways were favored by changing the electrocatalyst morphology (cubes or octahedra) and substituting Cu centers for Au nanospheres, synthesizing Cu2O-Au nanoparticles. Present efforts are to determine the liquid product distribution and investigate light irradiation.

Abstract:
Allied to the growing global energy demand, the increase in the global average temperature, mainly attributed to the high CO2 emissions from the burning of fossil fuels, brought impacting consequences to the planet. In order to alleviate both problems simultaneously and boost the use of sustainable means of obtaining energy, the electrochemical reduction of CO2 to higher value-added products, such as ethylene and ethanol, is proposed. This reaction has been studied since the middle of the 20th century and still has knowledge gaps that prevent its application on a large scale, such as the low yield and selectivity for the synthesis of C2+ compounds. In recent decades, the plasmonics branch has emerged as a possible solution to macroscopic barriers. The possibility of manipulating the light stimulus in matter on a nanometric scale allowed the discovery of new reaction pathways that are not possible in purely electrochemical conditions or in non-nanostructured electrocatalysts, in addition to enabling more precise control of selectivity. The various possible mechanisms for plasmon-assisted electrochemical reactions, and the lack of detailed studies in the literature, make this field very promising. This project aims to unite the localized surface plasmonic resonance of Au with the selectivity of production of C2+ compounds of copper-derived electrocatalysts, such as Cu2O, to synthesize Cu2O-Au nanoparticles aimed at a detailed study of the plasmon-assisted electrochemical reduction of CO2. The long-term goal of CO2 reduction studies is to decrease both thermodynamic and kinetic limitations, enabling its application on a large scale.

RCGI Project number: 60

A metal-organic framework/grafitic carbon nitride composite as photocatalyst for CO2 reduction to methanol

Bruno Manduca, Renato S. Freire, Pedro Vidinha

Keywords: Photocatalysis, Metal-organic framework, CO2

Impact: With the eminent dangers caused by climate change, it is imperative to reduce the CO2 concentration in the atmosphere. In nature, photosynthetic organisms utilize water and solar radiation to convert CO2 in organic species. With that inspiration, this work aims to study a metal-organic framework/graphitic carbon nitride composite to reduce CO2 using H2O and light. This is an easy and green process to both decrease de CO2¬ concentration and produce valuable chemicals.

Highlights: In the present work, methanol was produced from CO2, water, and visible light, without the utilization of any other reagent or sacrificial agent. The NH2-MIL-125(Ti)/g-C3N4 composite showed a better yield than the pure materials, namely 14,31 µmol g¬-1.

Abstract:
Photocatalytic CO2 reduction is an interesting strategy to address the global warming issue. Applying solar energy to convert CO2 into valuable chemicals and fuels is a promising process to reduce this gas atmospheric concentration while generating commercial products. A composite with titanium-based metal-organic framework (MOF) NH2-MIL-125(Ti) and g-C3N4 was synthesized by a facile deposition method. The material has been investigated for promoting photocatalytic reduction of CO2 under visible light in presence of water as sacrificial electron donor. The results show this system was able to produce methanol with a yield of 14,31 µmol g¬-1 under 10 MPa of CO2. The composite showed a better conversion than the materials NH2-MIL-125(Ti) and g-C3N4 alone, indicating a synergetic effect between them. The high specific surface area of NH2-MIL-125(Ti) and its amino groups facilitate the CO2 adsorption. The electron transfers to Ti atoms could explain the decrease of charge recombination when compared to pure g-C3N4. Higher pressure seems to promote the formation of methanol over other products like formate and methane. The present work provides a new approach for the application of MOFs in photocatalytic CO2 valorization.

RCGI Project number: 63

Conversion of ethanol to chemicals using rhenium oxide catalysts

Bryan Alberto Laura Larico, Liane Marcia Rossi, Lucia Gorenstin Appel, Laís Reis Borges, Danielle Kimie Kikuchi

Keywords: Rhenium, Ethanol upgrading, Heterogeneous catalysis

Impact: The studies involved in the discovery of new means of producing fuels are essential in the current world scenario, which is increasingly immersed in energy demands and the need to control global warming. Therefore, our work aims to advance in the study of new means of energy production (fuels) from ethanol, collaborating in the global effort to obtain energy from molecules other than oil.

Highlights: In this work we highlight the use of rhenium, a metal that has been insufficiently researched in the catalysis of ethanol, which in preliminary results showed that it has the ability to open new possibilities in obtaining chemical precursors for fuel production. Therefore, it is a metal that has potential for study.

Abstract:
"The increase in demand for renewable energy in Brazil and worldwide is a major concern today, which has caused an intensifying search for eco-friendly energy sources as a consequence of the inevitable exhaustion of petroleumbased fuels, in addition to the problem of global emissions of CO2 that have increased considerably in the last 30 years. These problems have directed the scientific community to study the conversion of CO2 into other products, such as hydrocarbons, alcohols, and others. Of these products, ethanol stands out as a chemical platform molecule, i.e., it is a precursor for several chemicals such as ethane, ethene, acetaldehyde, propanone, propene, butadiene, and others. In order to obtain the products mentioned above, the use of catalysts is necessary, so that the reaction is directed to the preferential formation of a desired product. In the literature, several catalysts are found for the transformation of ethanol into other compounds. Among the metals used in this catalytic reaction are copper, zinc, aluminum, and others. However, we observed that there is almost no research involving rhenium catalysts in the conversion of ethanol into other compounds. This metal has already shown promise in previous studies of our group, converting CO2 into methanol with high conversion and selectivity, in scientific literature is still reported the use of rhenium in the conversion of methanol into acetic acid, besides a patent with rhenium catalyst on zeolite ZSM5 for direct conversion of ethanol into propene. Thus, studies were performed with rhenium oxide catalysts supported on zirconium oxide (zirconia) and zinczirconia. Preliminary catalytic results showed that rhenium altered the catalytic activity of zirconia, increasing the selectivity for acetaldehyde by more than 30% at temperatures in the range of 200C to 350C, and decreasing the majority selectivity for ethane in pure zirconia. This is interesting because of the importance of acetaldehyde, which is an intermediate molecule for several other products of high interest, such as butadiene, propene, and others. So there is potential in using rhenium for converting ethanol into high value-added products."

RCGI Project number: 63

The influence of the Si/Al ratio on the formation of mesopores in SSZ-13 zeolite by the treatment with NH4HF2

Phd student José Henrique Marques and advisor Professor Dr. Leandro Martins

Keywords: MTO, Mesopores formation, Si/Al

Impact: Ethylene and propylene are two of the most used building blocks in the chemical industry. Currently, they are majorly produced by steam cracking of fossil sources. Alternatively, olefins can be produced by MTO reaction. Methanol can be produced from CO2 and biomass. The abstract presented concerns the improvement of catalysts used to methanol to olefins as a way of reducing the carbon footprint of goods produced from these building blocks.

Highlights: Methanol to olefins reaction can be used as a strategy to reduce the carbon footprint of olefins production. The catalyst suffer with deactivation by coke deposition and the creation of mesopores can improve the products diffusion. The treatment of SSZ-13 zeolite with ammonium hydrogen difluoride has shown different behavior to different Si/Al ratios (10, 20 and 40). The volume of mesopores alone is not able to dictate the behavior of catalyst in MTO reaction.

Abstract:
The fabrication of products with a lower carbon footprint has been sought to mitigate global warming. Methanol is a very important building block in the industry, widely used in various reactions, such as the production of formaldehyde, acetic acid, biodiesel, etc. Currently, methanol is mainly produced by synthesis gas, which can also be made from CO2, thus playing a very important role in the CO2 recovery chain. The zeolitic catalysts can convert methanol into gasoline and olefins in the MTG and MTO reactions. Deactivation by coke deposition is one of the biggest limitations of these processes, especially in the MTO reaction, due to the diffusional restrictions that the small pore openings play. Hierarchical catalysts can mitigate deactivation by coke deposition. One way to prepare these hierarchical catalysts is through treatment with NH4HF2 solution. It consists of removing silicon and aluminum atoms from the zeolite lattice, forming mesopores. It has been gaining much attention in recent years due to its alleged ability not to be limited to certain structures and Si/Al ratios. Thus, the present work aims to study the influence of the Si/Al ratio of SSZ-13 zeolite on the formation of mesopores by treatment with NH4HF2 solution. The SSZ-13 zeolites were prepared with different Si/Al ratios (10, 20, and 40) and submitted to NH4HF2 treatment. All samples maintained the CHA structure. The untreated samples showed micropore volumes of approximately 0.21 mL g-1 and non-relevant amounts of mesopores. The treated ones, in turn, had micropore volumes of 0.125, 0.165, and 0.080 mL g-1 and mesopore volumes of 0.159, 0.116, and 0.130 mL g-1, respectively. By BJH distribution of pores, the treated sample of ratio 40 showed mesopores centered at approximately 7.5 nm while at 20 and 40, above 20 nm. The treatment led to an increase in the Si/Al ratio in the samples. An increase in ethylene and propylene yield was obtained in the MTO reaction by treatment of Si/Al 40 zeolite, while in 10 and 20 ratios, there was a worsening. The treatment does not seem to behave equally in the different samples, requiring further investigation.

RCGI Project number: 63

Adequacy assessment of CO2 satellite measurements for Central Amazonia

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Keywords: Greenhouse gases, carbon dioxide, methane

Impact: In a world facing climate change it is important to know the carbon cycle and the role of greenhouse gases in the Tropical Forests as Amazonia Forest which stores 120 PqC in its ecossystem. GHG monitoring at surface are sparce in that region and satellite measurements can be an alternative to measure the gases concentrations with higher spacial resolution, bringing knowledge about Amazonian GHG concentrations.

Highlights: It is important to know GHG concentrations from Amazonia forest that is carbon sink, storing 120 PgC. To monitor this atmospheric concentration we can use in situ and on orbit measurements, but sensor measurements need validation. Thus, this work proposes to evaluate the adequacy of CO2 satellite products for central Amazonia.

Abstract:
"With the increase of the greenhouse gases concentration in the atmosphere in the last decades, monitoring and observing its sources and sinks became even more important, due to their impact in the earth climate and to the whole humanity, consequently. The first locations to perform CO2 concentrations measurements started at 1957 at the South Pole Observatory (SPO) and 1958 at Mauna Loa (Hawaii). Nowadays, this type of measurement occurs in different places around the world, such those at Total Carbon Column Observing Network (TCCON), counting with 26 sites in operation, however none in South America. Another way used to monitor GHG concentrations it is using orbiting sensors that even with their limitations like to present mean concentrations along the atmospheric column instead surface concentrations, they are not sparce like those in situ. Satellite concentration measurements to be consider need regular validation against independent in situ measurements. Thus, in the context of the atmospheric GHG concentration enhancement and climate feedbacks, Amazônia Forest plays an import role, acting as a carbon sink and storing 120 PgC in its ecosystem. However recent studies have pointed to a possible change in this scenario, due to climate change and forest degradation, in which it would be starting to be a source of carbon for the atmosphere.
"

RCGI Project number: 64

CO2 and SO2 Capture by Deep Eutectic Solvents: vibrational spectroscopy and DFT calculations

Giovanni Rodrigues Morselli, Pedro Henrique de Paula Sabanay, Rômulo Augusto Ando*

Keywords: Deep eutectic solvents, Raman, infrared

Impact: The characterization of the interactions of CO2 and SO2 with deep eutectic solvents is fundamental for the design of efficient processes for the capture, conversion and recovery of the absorbing solution.

Highlights: Raman and infrared spectroscopies are used to infer about physical and chemical interactions of CO2 and SO2 with different DES.

Abstract:
"The neoteric class of Deep Eutectic Solvents (DES) has been highlighted as the evolution of Ionic Liquids due to having many of their advantages as extreme-low vapour pressure, high chemical stability and the possibility to modulate their chemical properties by combining different cations and anions, while exhibiting simplified preparation, lower cost, higher biodegradability and lower toxicity. DES are generally prepared by the mixture of a salt with a hydrogen bond donor (HBD) at the specific molar ratio in which occurs the “deep” reduction of the mixture melting point. The HBDs in DES are generally compounds with functional moieties as amine, amide, alcohol and carboxylic acid. Among several applications of DES in green technologies as organic reaction media, extraction and nanotechnology, the capture of pollutant gases has been studied in order to reach a more efficient processes and to amplify the possibility of in situ conversion. Nowadays, sulfur dioxide (SO2) and carbon dioxide (CO2) are the main studied gases due to the urgency of the socio-environmental issues associated with them. SO2 is a polar and amphoteric gas that tends to interact with anions through charge transfer specific interaction, leading to high absorption capacities presented by DES and ionic liquids. CO2 is a nonpolar acidic gas that usually shows weak interactions with solvents, but presents chemical affinity with few species as amines, carboxylic acids and a special class of compounds known as superbases, which are unstable in its pure form, but stable within the DES. The interactions between CO2 and these species are of chemical nature, yielding carbamates or carbonates. In our project we aim to investigate interactions between the aforementioned gases and DES through vibrational spectroscopy techiniques as infrare and Raman, supported by DFT calculations. In this work, mixtures of reline or tetralkylammonium halides with SO2 were investigated through Raman spectroscopy and charge transfer interactions were evidenced by the downshift of the symmetric stretching band of SO2, vs(SO2). The extent of the charge transfer from the anion to SO2 enhances from chloride to iodide in mixtures of tetralkylammonium halides with SO2. In the case of CO2, DES formed by HBDs that are reactive towards CO2 are being currently investigated by vibrational spectroscopy. Moreover, in collaboration with Prof. Reinaldo Bazito group, new DES with superbases are going to be prepared and tested for CO2 and SO2 absorption.

"

RCGI Project number: 68

The methodology developed by the RCGI advocacy group to collect quantitative and qualitative data in climate change themes

LEMOS, Geraldo Lavigne de, ESLABÃO, Andrieza de Aquino, COSTA, Hirdan Katarina Medeiros, FAGÁ, Murilo, MOUTINHO DOS SANTOS, Edmilson. (All authors affiliation: USP)

Keywords: Methodological development, climate change, innovation

Impact: The methodology identifies promising solutions to address the challenges related to climate change, mitigation projects and adaptation strategies. The methodology was successfully tested with researchers of Greenhouse Gases, Nature-based Solutions, Carbon Capture and Utilization, Bioenergy with Carbon Capture and Storage. The methodological development presented proved successful and the model may be replicated in similar cases of other researches.

Highlights: The developed methodology may address climate change challenges. The methodology was tested with researchers of climate change related themes and proved to be successful to (i) obtain quantitative and qualitative data, (ii) summarize long-term experiences, (iii) aggregate sparse data, (iv) support solutions and policies to face climate change, and (v) identify stakeholders, regulatory gaps and implementation difficulties.

Abstract:
The challenges related to climate change, mitigation projects and adaptation strategies requires innovative remedies. This article aims to present a methodology to identify promising solutions to address those issues. The development of this methodology consisted in the preparation and application written forms, followed by the realization of workshops. The written form was initiated with the elaboration of a preliminary form, submitted only to the members of the advocacy group of the Research Center for Greenhouse Gas Innovation (RCGI), in order to test the preliminary form and, thus, support the preparation of the final form. In this context, the preliminary form gave rise to the assessment of the clarity of the questions and the usefulness of the answers, considering that it must collect data to be categorized, systematized and analyzed from a scientific point of view. After the application of the preliminary form, the members of the advocacy group were invited to participate in a feedback meeting to present their critical analysis of the form as respondents. Such measures allowed the improvement of the preliminary form to prepare the final form. Then, the final form was submitted to researchers of the interest areas, taking place the initial data collection. After that, the same researchers were invited to participate of workshops, especially useful to collect specialized and qualitative data from those researchers. To combine written forms with workshops was essential to optimize the data collection. The methodology was successfully tested with researchers of Greenhouse Gases, Nature-based Solutions, Carbon Capture and Utilization, Bioenergy with Carbon Capture and Storage. The test proved the effectiveness of the written form combined with the workshop to obtain quantitative and qualitative data, summarizing the long-term experiences of different researchers. The methodology developed supported to aggregate sparse data and to obtain crucial information for the improvement of solutions and policies to cooperate with mitigation projects and adaptation strategies in a climate change scenario. In addition, the methodology developed enhanced the identification of stakeholders, regulatory gaps and implementation difficulties. The methodological development presented proved successful and the model may be replicated in similar cases of other researches.

RCGI Project number: 69

State of the art of carbon capture in the industrial sectors: an overview

Celso da Silveira Cachola, Alex Azevedo, Mariana Ciotta, Drielli Peyerl

Keywords: Carbon capture, Greenhouse gas emissions, Industrial sectors

Impact: Knowing the industry sectors with the greatest propensity for carbon capture allows us to understand the places with the potential for adopting or commercialising carbon capture technologies.

Highlights:
- There are several industrial sectors with potential for implementation carbon capture technology, mainly iron and steel production and cement manufacturing.
- There are also several carbon capture technologies that can be used in the industrial sectors, such as etanolamine (MEA) or metildiethanolamine (MDEA) post-combustion and chemical looping.

Abstract:
The climate crisis is one of the most critical global problems arising mainly from greenhouse gas (GHG) emissions. Considering GHG emissions from industrial processes, one of the leading technological alternatives to achieve the net zero carbon goal is carbon capture. Carbon capture will play an essential role in the future energy transition, so it is crucial to understand the key industrial sectors where these technologies could be deployed. Therefore, this work aims to identify and analyze the main industrial sectors that have the potential to deploy carbon capture globally. A systematic literature review was carried out, followed by bibliometric analysis. The methodology followed three steps: (i) performing an advanced search in the Scopus database with the primary descriptors “carbon capture”, the acronyms CCS - abbreviation of carbon capture and storage - and CCUS - abbreviation of carbon sapture, utilization and storage -, and “industrial sectors”, (ii) analysis of the papers' abstracts with the support of the Rayyan web application, and the analysis had as a guiding question: does the scope of the analyzed paper contain any industrial sector in which carbon capture can be applied?, and (iii) identify which industrial sector was contained in the analyzed paper. The research was conducted on May 2, 2022, finding 58 papers. Following step (ii), only 20 papers were selected, since these papers answered the guiding question of this work. After performing the three methodological steps and analyzing the results found, iron and steel production was the industrial sector with the highest number of papers - 13 papers -, followed by cement manufacturing - 8 papers -. Following iron and steel and cement, the most important sectors were: energy generation, that is, power plants - 6 papers -, chemical products - 5 papers -, pulp and paper mills and fuel refineries - 2 papers in both sectors - and glass factories - 1 paper -. The efficiency and type of carbon capture technology used were also evaluated, and the data found varied by industry sector, with etanolamine (MEA) or metil dietanolamine (MDEA) post-combustion and chemical looping technology being frequently cited. The number of citations indicates that iron and steel production, followed by cement manufacturing, is the most advanced industrial sector in terms of scientific research on using carbon capture to reduce GHG emissions. However, the power generation, chemical, refinery, pulp and paper mills and glassworks sectors are also prone to carbon capture.

RCGI Project number: 70

Molecular storytelling on diffusion of low carbon society technologies

Dindara S. Galvão, Renan S. Sampaio, Caetano R. Miranda

Keywords: molecular storytelling, virtual reality, public perception

Impact: Immersive narratives at nanometer scales have great potential to improve materials design processes and also to improve the public perception of science, allowing the user to access scales that would not have access to in everyday life, materialising in people's imagination, very complex interactions that otherwise would be very difficult to explain in a didactic way.

Highlights: Experimentation of Molecular Dynamics simulations combined with virtual reality visualisation.
Production of screenplays and posterior recording of videos leading the user through these simulations in a didactic way.
Thoughts on the possibility of using molecular storytelling to improve public perception of science and discuss solutions to global problems.

Abstract:
Immersive experiences through Virtual reality (VR) and Science & Art intersections can be an exciting and attractive tool to improve public perception on energy transition and climate change issues. By combining Molecular Dynamics and VR, it was possible to immersively visualise systems at nanoscale of interest on low carbon technologies. The systems explored were : i-) lithium in aqueous solution, ii-) carbon nanotubes, iii-)boric acid in nanopores in a graphite sheet, iv-) porous metal-organic structures (MOF) formed by zinc ions with an organic ligand through while CO2 is diffusing. All simulations were modelled using PACKMOL and LAMMPS provided by the SAMPA group at IFUSP. The software NOMAD VR was used to enable the visualisation and lets the user to view the systems in VR glasses and smartphones. Oculus rift was used, which allows the user to navigate through the structures with the controllers, trigger and pause the movement of molecules. One can create an intuition on how molecules behave and interact over time. The perception of the user of the glasses was replicated to the computer screen by Oculus Mirror software. This set-up enables the possibility to record in 2D the user path during the immersive experience. Interviewing the members of the SAMPA group who produced and provided the simulations, it was possible to identify the most relevant parts of each system, and propose more creative and didactic ways of conducting the viewer through them. Culminating in the production of four screenplays, one for each structure, of best ways to record the experiences. Videos were recorded that navigate through each molecular system, highlighting important details of their configuration, both statically and dynamically, following the inter and intramolecular interactions and how the arrangement changes over time. The video content production can help expand access to the perception of nanometric scales, even in circumstances where virtual reality glasses are not available. Molecular Storytelling has a big potential to change the public perception of science, using the best route to, artistically and educationally, perceiving and understanding complex molecular processes as well as benefiting the design of new materials, and also in solving global issues such as environmental problems related to the mitigation of greenhouse gases. The possibilities are endless.

RCGI Project number: 70

Design and optimization of centrifugal compressors operating with carbon dioxide and mixtures of methane and carbon dioxide

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Keywords: Centrifugal compressor, design, optimization

Impact: Centrifugal compressors are important for the extraction and transportation of carbon dioxide and methane. Developing technologies specific to these applications enhances the efficiency of the compressors, reducing costs and CO2 emissions.

Highlights:

- Application of the meanline method for mixtures,
- Optimization of the geometrical parameters based on the meanline method
- Optimization of the streamlines by designing the channel of the compressor based on a 2D method
- Full 3D simulation of the optimized centrifugal compressor

Abstract:
The good performance of centrifugal compressors depends fundamentally on a good design. Even with the technological advances of recent decades, this project is still carried out through one-dimensional tools, since they are much faster than three-dimensional tools and present reliable results, being able to estimate geometric parameters, thermodynamics, and flow speeds in the compressor, so that it is possible to determine the performance parameters as pressure relations, isentropic efficiency and required power. This research project aims to implement one of these one-dimensional methodologies, the meanline method, in computational code to develop a tool capable of designing and predicting the behavior of centrifugal compressors for working fluids that have been little explored in the open literature. Carbon dioxide and mixture of carbon dioxide and methane were chosen due to their relevance in the present context. The thermodynamic properties of the fluids studied are calculated from the REFPROP library, and the equations of state used for carbon dioxide are based on Span and Wagner (1996) and for the mixtures on Kunz (2012). With the validated program, a genetic optimization algorithm, NSGA-II, was coupled to the said program, with a mutation operator equal to 0.9 and the crossover operator equal to 1.0 to minimize the chances of the process being restricted to local minimums and with the initial population used in the optimization process generated through the Latin Hypercube Sampling method. The objective function of the optimizer is to maximize the isentropic efficiency and to develop a centrifugal compressor optimized for work in its real operating conditions. The optimized geometry will be submitted to a 2D methodology for the optimization of the streamlines and the channel of the compressor. The working conditions of the compressors to be developed for the mixture of methane-carbon dioxide will be the Cortez pipeline located in the USA and considering the supercritical conditions of 316 K and 18.6 MPa. The compressors developed using 1D and 2D optimization will be submitted to a complete 3D CFD simulation using the Ansys CFX program to verify the validity of the 1D and 2D optimization and the loss functions and to understand the phenomena that occur in the compressor

RCGI Project number: 72

Software development for inverse problems in time domain acoustic wave propagation using higher order finite elements

A. Olender, T. dos Santos, D. Dolci, B. S. Carmo

Keywords: Full waveform inversion, higher-order mass lumping, finite element modeling

Impact: This work focuses on extending an open-source software implementation for solving full waveform inversion (FWI) problems. FWI is commonly used in geophysical exploration studies, but it has applications in surveying carbon capture and storage sites, noninvasive neuroimaging and high-resolution ultrasound breast imaging.

Highlights:
*Addition of support for 4th order mass lumped tetrahedral elements with unstructured meshes.
*Sparse interpolation and injection extended to high-order quadrilateral elements.
*Added functionality to support ongoing implementations of multiscale FWI with adapted remeshing, usage of the elastic FWI together with moving meshes, automatic adjoints, source encoding, and weight-adjusted DG elements.

Abstract:
In this work we present improvements in an open-source software stack focused on solving wave propagation in heterogeneous domains and performing full waveform inversion (FWI). The current software is capable of finite element discretizations for wave equation in 2D and 3D using triangular and tetrahedral meshes together with higher-order mass lumping, and quadrilateral meshes with spectral finite element methods. The usage of triangular elements enables studies involving unstructured waveform adapted meshes with results presented in complex realistic geophysics examples. We also demonstrate initial results of the newer software implementations.

RCGI Project number: 46

Rio Bonito Formation suitability for permanent CO2 storage

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Keywords: Geological carbon storage, CO2 storage site characterisation, Rio Bonito Formation

Impact: By analysing reservoir and sealing quality, leak risks, data coverage, available infrastructure in the region proximity, and the social context, this work indicates that Rio Bonito Formation presents a promising opportunity for permanent CO2 storage in Brazil, mostly in term of its strategic location and adequate petrophysical characteristics for storage capacity and containment.

Highlights: The reservoir quality of the sandstones indicates sufficient storage capacity and petrophysical reservoir properties, especially due to average depth and thickness.
The presence of mudstone layers suggests a promising sealing quality, with low seismicity activity.
Regional proximity analysis showed good accessibility to potential sites for CO2 injection, considering its onshore location and the great concentration of stationary CO2 emitting sources.

Abstract:
Carbon Capture and Storage technologies (CCS) are one of the key tools for the required reduction of greenhouse gases in order to meet sustainable development scenarios to limit the climate change harmful effects. Geological carbon storage plays an essential role in the deployment CCS technologies worldwide at scale. Finding the suitable geological units for CO2 storage requires interdisciplinary studies that must be addressed to each potential injection site. Considering a field-based approach, an initial site screening for CO2 storage in the Rio Bonito Formation in the Paraná Sedimentary Basin was performed in this work, in order to identify its suitability for permanent CO2 storage. Main parameters and properties related to reservoir quality, sealing quality and other leak risks, data coverage, regional proximity analysis, and social context analysis were compared to desirable characteristics for site selection. The analysis suggests a good potential of petrophysical available data for storage capacity and indications of effective containment of the injected CO2 due to the presence of mudstone layers. However, it is required further characterization of the geological system and trapping mechanisms and assessments of public perception on CCS in the region.

RCGI Project number: 58

Enhanced electrochemical reduction of N2 with materials of plasmonically active metal nanoparticles, (Au, Ag, Pd, Ru) and (Mo, Ti, Ce), combined with n-type semiconductors.

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Keywords: N2 Electrocatalytic reduction, Metallic Nanoparticles, Mechanochemistry

Impact: Obtaining ammonia is currently carried out through the Haber-Bosch process with the consumption of Nitrogen and hydrogen, this process includes a high energy consumption, at high pressures and temperatures. Electrocatalysis provides a way to obtain ammonia through nitrogen, which does not require such extreme working conditions, assuming a solution for this issue. Provides the use of novel eletroative materials of metallic and bimetallic nanoparticles with morphologies conditioned for Nitrogen fixation.

Highlights: The search for electroactive materials that have an affinity for nitrogen fixation on their surface, conditioning the breaking of the triple bond of the molecule and its easy reduction, is a challenge in this research. In this work, porous materials of metallic and bimetallic Gold and Silver nanoparticles are shown that show electrocatalytic activity for the system in question.

Abstract:
"Obtaining NH3 is of marked importance due to its applicability today. Ammonia serves as the basic starting material for synthetic fertilizers rich in nitrogen, a very important aspect of agriculture. In the industry, the Haber-Bosch method is proposed as the most accepted for obtaining it. This process has several disadvantages since it is necessary to consume high amounts of energy, high pressures, and at temperatures between 300-500 °C, by using nitrogen and hydrogen to obtain ammonia with very low yields and results. Thus consuming 2% of global energy consumption.
Currently, electrochemical processes are being reported to obtain this compound, using different catalytic systems. In this field, nanoscience has made great advances, providing improvements in the performance and speed of obtaining compounds. In this work, the study of obtaining ammonia through the electrocatalytic reduction of N2 is proposed, using materials of metalorganic morphology with metal nanoparticles such as Ag, Au(Ag@ZIF8,Au@ZIF8, AgAu@ZIF8,) and the combination of these, using electrolytes of various nature.
"

RCGI Project number: 60

Effect of rhenium precursor and composition on the catalytic performance of ReOx/TiO2

Felipe Machado (IQ-USP), Pedro Vidinha (IQ-USP) e Maitê Gothe (IQ-USP)

Keywords: heterogeneous catalysis, CCU and supercritical fluid

Impact: From this work, the objective is to develop methodological strategies for scaling up the ReOx/TiO2 catalyst, patented by the research group, for industrial applications. However, some challenges must be overcome, given the complexity of the variables in the scheduling of industrial catalysts, such as choosing a course with good cost benefit and excellent catalytic performance, in addition to maintaining the results on a bench scale in a semi-industrial scale. As well as the preparation of molded catalytic supports, which will be prepared and studied in future works by the group.

Highlights: The choice of active metal precursor can influence catalytic performance. With this, it can be better understood that the main agent responsible for the conversion of CO2 to methanol would be ReOx or metallic rhenium. Furthermore, there is a possibility that the type of rhenium oxide affects the oxide reduction due to different type of interaction with the support.

Abstract:
Humanity today has the great challenge of reducing greenhouse gas emissions, especially CO2, as soon as possible in order to avoid an irreversible catastrophic climate scenario. The challenge becomes more arduous when the limit of the planetary boundary related to the variable climate change has already exceeded the safety limit to maintain the self-conservation of the Earth system. One of the causes of this extrapolation is the high concentration of CO2 in the atmosphere. To minimize these damages, experts believe that carbon neutrality would be a good alternative. Carbon neutrality is a state of net zero emission of CO2 that many nations aim to achieve by 2060 at the latest. Scientists around the world have developed promising technologies for capturing, storing, and converting CO2 into carbon added value products with the view to achieve the CO2 emission reduction targets under the Paris Agreement. Among these, carbon capture and utilization (CCU) technologies have been gaining prominence for their potential to generate value-added chemical compounds and promote a circular carbon economy. This work uses CCU technology to convert CO2 to methanol through catalytic reduction reaction with H2 and ReOx/TiO2 catalysts. The objective of the present work is to evaluate the effect of changing the Re metal source precursor and its composition on the support surface (TiO2) on the catalytic performance, in terms of conversion and selectivity. For this, 100 mg of TiO2 were wet impregnated with the precursors NH4ReO4 and Re2O7, with enough mass for nominal loading of active metal between 5, 10 and 20 wt%. After impregnation the samples were pre-reduced to 500°C between 1 and 2h. Then, the catalytic tests were performed in batch with the molar ratio 1 mol CO2/1 mol H2, P = 100 bar, T = 200ºC, 10 mg of catalyst and 16 h of reaction. Previously, the reaction samples were reduced in-situ to eliminate possible rhenium oxides formed after pre-reduction by exposure to atmospheric air. Finally, with regard to understand some properties of the catalysts, they were subjected to the following characterization techniques: X-ray diffraction, Rietveld refinement, Raman Spectroscopy, Fourier Transform Infrared Spectroscopy, Inductively Coupled Plasma Atomic Emission Spectroscopy and surface area determination by the BET method.

RCGI Project number: 63

Development of Catalysts for the Direct Conversion of CO2 into Higher Alcohols

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Keywords: CO2, cobalt, alcohols

Impact: The high concentration of CO2 in the atmosphere due to the utilisation of fossil fuels over the years has resulted in serious environmental problems throughout the globe and thus should be addressed properly and immediately. The development of catalytic systems for the conversion of CO2 into value-added chemicals such as higher alcohols offers a plausible pathway towards a greener future.

Highlights: In this work, we observed that modifying the structure of Co-based catalysts by adding dopants can alter CO2 conversion and selectivity of such catalysts in CO2 hydrogenation reactions. The formation of CO, CH4 and higher alcohols are profoundly influenced by the precursors and synthesis method.

Abstract:
"The global emissions of CO2 and, consequently, its adverse effects have increased considerably over the past years, especially as a direct consequence of the huge consumption of fossil fuels. So as to address such issue, the CO2 conversion into valuable chemicals has gained greater attention as a feasible solution [1], whereby the the reverse water-gas shift (RWGS) reaction and the Fischer-Tropsch synthesis (FTS) are coupled in order to produce a plethora of compounds [2]. Co-based catalysts have been proven to be excellent for FTS of syngas (CO + H2), being capable of yielding long-chain hydrocarbons even at relatively low temperatures. Such characteristic can be attributed to various factors such as high turnover rates and high chain growth probability [2]. The CO2 hydrogenation over cobalt-based catalysts, nevertheless, still poses a major challenge by virtue of the lack of structure controllability and hurdles linked to tuning the products selectivity deriving from the nonexistence of fundamental comprehension over mechanistic routes [3]. Over the gamut of probable compounds obtainable from CO2 hydrogenation, ethanol has been keenly sought and studied since it can be utilised as solvent, additive and precursor for other reactions. However, there are still serious impediments to this reaction, such as C-C couplings as a result of dissociative and non-dissociative CO, in addition to the adsorption and activation of CO2 [4]. Aiming at overcoming such problems and expanding the comprehension of such catalytic systems, we synthesised Co-based catalysts so as to undergo CO2 hydrogenation reactions. Aiming at overcoming such problems and expanding the comprehension of such catalytic systems, we synthesised Co-based catalysts so as to undergo CO2 hydrogenation reactions. In this work, we investigated how the addition of promoters to cobalt-based catalysts affects the formation of higher alcohols in hydrogenation reactions under high pressures. Therefore, we offer insights into how reaction parameters such as temperature or dopants addition may preferentially favour catalytic pathways such as RWGS or FTS.
[1] Appl. Catal. B., vol. 315, p. 121529, Oct 2022
[2] Appl. Catal. B., vol. 305, p. 121041, May 2022
[3] Chem. Eng., vol. 446, p. 137217, Oct. 2022
[4] Chem. Eng., vol. 433, p. 134606, Apr 2022"

RCGI Project number: 63

Synthesis and Characterization of Porous Carbon Materials as Catalysts for CO2 Hydrogenation

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Keywords: Carbon Porous, CO2, Catalyst

Impact: The increase in human activities since industrialization has raised the global concentration of CO2 in the atmosphere at an alarming rate. To mitigate this trend, it is necessary to develop economically viable technologies for capturing and converting CO2. Therefore, the study of carbon-based materials constitutes a strategy for the discovery of catalysts to convert CO2 into value-added products.

Highlights: This work aims to use the pyrolysis of ZIF-67 impregnated with metals as a way to synthesize porous carbon materials as catalysts in the hydrogenation of CO2. At the present moment, this project is in an initial stage of development, where a screening is being carried out on which dopants can favor the formation of value-added products in CO2 hydrogenation.

Abstract:
"With the COVID-19 pandemic, significant challenges for the energy transition have been created. The emphasis on economic recovery from the cost of progressing the energy transition raises concerns around the world.[1] Thus, the use of fossil fuels is still present, which contributes to increased CO2 emissions and, consequently, generates environmental impacts. Carbon materials are extremely versatile, exhibiting applications in thermal, electro- and photocatalysis.[2] Besides, such materials have been promising candidates for CO2 hydrogenation reactions. Few studies have focused on elucidating mechanisms and synergistic effects in these systems, and the effect of promoting selective hydrogenations is still a challenge. The pyrolysis of metal-impregnated ZIF generates porous carbon materials with intermetallic phases, which have high selectivity in CO2 conversion.[3] This work aims to use the pyrolysis of ZIF-67 impregnated with metals as a way to synthesize porous carbon materials as catalysts in the hydrogenation of CO2.

References:
[1] Appl. Energy, 2022, 307, 118205.
[2] Mater. Adv., 2020,1, 1506-1545.
[3] Eur. J. Inorg. Chem., 2021, 44, 4521-4529."

RCGI Project number: 63

Experimental validation of labyrinth seals designed by topology optimization

Lucas Neves Braga Soares Ribeiro

Keywords: Otimização Topologica, Selos labirinto, Validação experimental

Impact: To reduce leakage is one of the key goals to reducing greenhouse and F-gases emissions, so Topology optimization is one great tool for designing better seals. One of the main processes of the design is experimental validation, so we can ensure that the improvement is measurable and real.

Highlights: Design and built two different test benchs for experimental validation of labyrinth seals.
Able to evaluate the leakage with and without rotation, in '3D' or '2D' models.

Abstract:
This project is part of the research 'Design of Smart Labyrinth Seals for Mitigation of GHG emissions in pneumatic machines (compressors and turbines)" on gas emission reduction of the greenhouse effect at the Research Center for Greenhouse Gas Innovation (RCGI). A great part of these emissions is related to the leakage that occurs in systems of compressors, turbines, and rotating machines, between the fixed part and the rotating part of these devices. To mitigate these leaks, it is common to use labyrinth seals, a type of non-contact annular mechanical seal, which normally use flow restrictions and cavities to reduce these leakages. It is proven that leakage reduction can be achieved by changing the geometry, therefore recent studies have been carried out on labyrinth joint geometries designed using topology optimization. A mathematical method that optimizes the distribution of material within a given design space, for a given boundary condition and constraints with the objective of maximizing its performance, in this case, reducing the leakage flow. This research carries out the complete development cycle of a labyrinth joint designed by topology optimization. An algorithm developed by the research group will be used to obtain the project concept of the labyrinth seals and then the post-processing of this project will be carried out conceptual. The labyrinth seal will be manufactured through additive manufacturing and then validated experimentally. In the literature, there are few experimental works on labyrinth seals and there are few studies that carry out the experimental validation of components designed using topology optimization, including the design and construction of a test bench to be used in the experimental validation of labyrinth seals prototypes. Therefore, this research seeks to contribute on these two fronts.

RCGI Project number: 65

Greenhouse gases adsorption in ZIF-8 via first-principle calculations

Matheus Finamor, Carlos Alberto Martins Junior, and Caetano Rodrigues Miranda

Keywords: Metal-Organic Frameworks, Zeolitic Imidazolate Frameworks, CO2 adsorption

Impact: The study of new materials able to capture carbon dioxide is essential for mitigating greenhouse gases emissions. This work is related with the Sustainable Development goals set up by the United Nations, more specifically, with goals 7 and 13, associated with affordable and clean energy and climate action, respectively.

Highlights: In this work we characterized a new class of mesoporous material regarding carbon capture. We calculated the energy of adsorption for CO2 at different adsorption sites with first principle calculations. These calculations help to validate classical Force Fields that predict very good selectivity for adsorbing carbon.

Abstract:
The emission of greenhouse gases by human activity leads to climate change, threatening life as we know it. Carbon dioxide (CO2) is one of main responsible for the increase in global surface average temperature. In that way, it is essential to capture and store CO2 efficiently, a strategy of mitigation known as Carbon Capture and Storage. With that, we can mitigate climate change without drastic changes in our economy. In this work, we study Metal-Organic Frameworks (MOFs) as a potential material able to capture CO2. These frameworks are very promising regarding carbon capture due to high surface areas, tunable pore size, and high potential for industrial-scale production. In particular, we study a specific MOF, the Zeolitic Imidazolate Framework 8 (ZIF-8). ZIF-8 is composed of zinc coordinated with imidazole, structured in cubic symmetry and sodalite framework. Calculations were performed based on density functional theory (DFT), as implemented on VASP package. The optB86b-vdW functional, which includes dispersion forces, has been used. We characterize CO2 adsorption in ZIF-8 by identifying different adsorption sites and their respective adsorption energy. The preferable site for CO2 adsorption is related to the organic ligands with adsorption energy of -0.35 eV. These calculations also help to validate force fields developed for classical calculations, indicating that they can capture the adsorption as it happens at quantum level. Moreover, recent experimental findings suggest that thermal post-treatment of ZIF-8 can enhance its carbon capture capability. Therefore, we modelled propositions of the role of defects induced by this kind of treatment and studied if it is stable, the formation energy, and how it would affect adsorption.

RCGI Project number: 68

What is going on with Carbon Capture and Utilization?

Leão, Clarissa, Motta, Karen. K. M., Nunes, Romário.C., Costa, Hirdan K. M., Silva, Isabela, Seabra, Paulo.N., Moutinho dos Santos, Edmilson.

Keywords: Carbon capture, CCU, CO2 emissions.

Impact: Carbon capture and use may seem incipient in the world, especially in Brazil. However, the IEA (2019) estimates that this market can reach at least 10 MtCO2/year for each potential segment, including fuels, chemicals, mineral building materials, waste construction materials, and fertilizers, in the short term. Given the great potential and multiplicity of CCU forms and the importance of technologies of this nature for the reduction of greenhouse gases, this article aims to answer the following question: why does this theme not seem to advance and develop in a relevant way in Brazil and the world?

Highlights: It is observed that there was a reduction in the complexity of the projects added to the climate objectives strengthened, generating a new "momentum" for the CCUS in the world (IEA,2021), which can be portrayed by the increase of 80% in the number of projects developed between 2010 and 2021 (IEA, 2021).
Finally, it is interesting to mention that the main CCUS projects developed in 2021 mainly occurred in Europe and the United States, representing a percentage between 30 and 40% (IEA, 2021).

Abstract:
"The use of CO2 in the advanced recovery of hydrocarbon reservoirs has been a recurrent practice in the oil industry for many decades (HINRICHS et al.,2014). This kind of capture and use of CO2, also called carbon sequestration, in Brazil, is regulated by The National Agency for Petroleum, Natural Gas and Biofuels Resolution No. 17/2015 (RANP 17).
In RANP 17, CCU would be a form of "advanced recovery" of oil. Advanced, optimized, or tertiary recovery occurs when CO2 is injected directly in the reservoir, so the pressure increases oil releases from the rock (HINRICHS, 2014).
Although tertiary recovery is one of the most advanced methods of CCU, this is not the only possible way to capture and use it. Industrial energy generation and consumption processes are alternatives to implementing carbon capture and subsequent use (COSTA, 2020, IEA, 2020). Therefore, the energy sector and the industrial sector are strong candidates for the adoption of CCU techniques, which can enable the reduction of their emissions through these technologies.
Capture can occur by various technologies, which depend directly on the issuing source (KUNZE, SPLIETHOFF, 2012). Capture technologies are constantly improving, but in general, they sequester carbon from stationary sources (FERON, HENDRIKS, 2005). There are already initiatives aimed at capturing carbon directly from the air. However, according to SILVA (2022), the economic viability of this capture will possibly come through carbon pricing, which can generate resources for investments in increasing the efficiency of this method.
The IEA (2019) explains that a consolidated CO2 market already consumes about 230 million tons of this product, whose primary use is in the fertilizer industry. A widespread and customary example of the use of carbon dioxide is in the food industry in carbonated beverages (ARESTA, DIBENEDETTO, ANGELINI, 2014). Similarly, capture studies on carbon use are constantly evolving, and new uses for the chemical industry, fuels, and building materials are a development and study front (PACHECO, 2021).
In this sense, to understand the reason for the CCU not advancing on a large and fast scale at the national and international levels, WANG et al. (2021) focused on the analysis of 263 carbon capture, utilization, and storage (CCUS) projects developed between 1995 and 2018. In the evaluation, the authors concluded that the risks associated with the development of CCUS projects were high, and for their reduction proposed (i) reduction of the capacity of each project, (ii) reduction of the deadline for

project development, (iii) government development support, and (iv) carbon tax and credit at high levels.

Similarly, the IEA (2021) understands that to accelerate CCUS projects, lower cost and less complex industrial projects should be implemented. According to the Agency, the reduction in the complexity of projects added to the strengthened climate objectives generates a new momentum for the CCUS in the world (IEA,2021), which can be portrayed by the increase in the number of projects under development.

Furthermore, in this sense, the IEA (2021a) points out three elements as indicators that the learning of recent years has created an environment conducive to the effective development of the CCUS worldwide. They are (i) recognition that the CCUS is necessary to achieve zero carbon targets by countries, (ii) international interest in the production of low carbon hydrogen, which would require the capture of CO2 in its production, and (iii) a new wave of incentive policies specific to this technology.

In Brazil, there are no robust discussions aimed at increasing investments in CCU. However, recently it was filed in the Federal Senate the Bill No. 1425 of 2022 (Bill 1425), which "Disciplines the exploitation of the activity of permanent storage of carbon dioxide of public interest, in geological or temporary reservoirs, and its subsequent reuse" (FEDERAL SENATE, 2022). This Bill is the result of four years of research by the Advocacy Group at the Research Centre for Greenhouse Gas Innovation (RCGI) of the University of São Paulo, financed by the Research and Development clause of Brazil's oil and gas concession contracts.

Although the Bill 1425 specifically brings legal certainty about the storage and division of responsibilities on CCS, there is complementarity between CCU and CCS since "the life cycle of CCU naturally integrates with the life cycle of CCS" (SILVA, 2022). Thus, in addition to bringing more legal certainty to the life cycle of carbon dioxide, the regulation of CCS can boost CCU.

Also, on the feasibility of CCU projects in Brazil in addition to the advanced recovery of oil, Decree No. 11,075, of May 19, 2022, "establishes the procedures for the elaboration of the Sectoral Plans for Mitigation of Climate Change, establishes the National System for the Reduction of Greenhouse Gas Emissions and amends Decree No. 11,003, 21, 2022" (BRASIL, 2022). This decree seeks to introduce a carbon market in Brazil, and, although it requires additional regulation and more significant efforts to realize the market effectively, this type of initiative can enable investments in new – or even existing and even in the study phase – forms of CCU, which will become economically viable by carbon pricing.

Final Considerations

Even though, in recent years, many CCU projects have been abandoned before their implementation, the current moment is favorable for developing projects of this nature. Due to ambitious carbon-neutral plans, several countries have promised vast investments in CCU, gaining prominence in the U.S., where billions of dollars are expected to fund this type of project in the coming years.

In Brazil, the advanced recovery of oil already occurs and is regulated by the ANP. In 2022, in addition to incipient initiatives for creating a carbon market, the National Congress is already analyzing a carbon capture and storage bill. Propositions of this nature may mean the feasibility of new forms of CCU in the country by (i) bringing the carbon dioxide industry to public debate and (ii) enabling investments in CCS for carbon pricing.

It cannot be categorical to state that the CCU chain will flourish in the coming years. However, the emergence of financing, new projects, and carbon markets may indicate that in the future, this market will prosper and more strongly support the reduction of greenhouse gases internationally.

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RCGI Project number: 69

Atlas of Low-carbon technologies and Hydrogen hubs for the Brazilian Descarbonization

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Keywords: Low-carbon technologies, Hubs, Map overlay method,.

Impact: Analyzing the feasibility of implementing low carbon technologies and building hydrogen poles in a region requires a large set of specific local information such as geographic, social and historical. In this work, a sociogeographic model was applied that uses the map overlay method that combines analytical layers to implement and/or build low carbon technologies and hydrogen hubs. Carbon Capture and Storage (CCS) will be the first example demonstrated.

Highlights:
- Cities with steel mills and close to the coastal region showed greater viability, especially Serra - ES and São Gonçalo do Amarante - CE,
- The use of port transport infrastructure and the geological potential of nearby oil fields boosted these hubs.
- Although geographically distant, these hubs are similar regarding recent industrialization, high gross GDP, poor income distribution and low social indices.

Abstract:
Accelerating the transition process to low-carbon technologies has become one of the key measures to achieving global climate goals. In this sense, the carbon capture and storage (CCS) technology holds great potential, as it can reduce emissions from existing facilities – such as power plants, refineries, iron and steel mills, and cement plants – and serve as an intermediate step in decarbonization or even be combined with disruptive technologies. Thus, this work aims to build a framework of geographic, social and historical information for CCS deployment potential in Brazil and later analyze possible locations for deploying CCS hubs. The methodology of this work consists of two steps: (i) advanced search in the Scopus database to find requirements necessary for deployment CCS, and (ii) elaboration of a correlation between geological potential, greenhouse gases (GHG_ emissions by sectors, and available infrastructure for transporting the captured carbon, such as pipelines and railroads. In the Brazilian case, data of GHG emissions were recoverd from the Greenhouse Gas Emissions Estimation System (SEEG), data on offshore storage of carbon dioxide (CO2) – acquired from scientific literature - , and data on transport infrastructure and gas pipelines – obtained from government companies, such as the National Petroleum Agency (ANP) and the Energy Research Company (EPE). Data processing was done in QGIS software, a tool which calculated the superposition of these layers, using the Map overlay method, allowing the analysis of the material. According to the literature, the main sectors for deployment of CCS are concentrated in the industry sector. Two possible main hubs were found in Brazil: (i) the municipality of Serra, in the state of Espírito Santo, and (ii) São Gonçalo do Amarante, in the state of Ceará. Both regions have high GHG emissions levels, mainly from iron and steel activities, and the infrastructure potential is associated with pipelines and railroads' proximity. Although geographically distant, the sociodemographic data present similarities, both municipalities had rapid economic expansion due to economic activity, resulting in accelerated population growth, an increase in gross income, and a drop in social indicators. Another similarity between the regions is the long-term projection of using hydrogen such a tool for decarbonization in the iron and steel sector. However, there are no current projects declared by the companies with CO2 emissions to significantly reduce emissions in the next ten years. BECCS and hydrogen will be added as study cases in the following steps of the Atlas.

RCGI Project number: 70

CO2 geological storage opportunity in basalts of the Paraná Basin (Brazil): Perspectives from CO2 mineralization processes in the Serra Geral Formation

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Prof. Dr. Colombo Celso Gaeta Tassinari

Keywords: CO2 geological storage, carbon mineralization, Paraná Basin

Impact: Given that Brazil remains on the list of countries with the highest CO2 emissions, it is important to implement technologies to address and mitigate climate change consequences. Carbon geological storage through CO2 mineralization in basalts has been proven in operational projects and offers the opportunity of injecting up to 1 Mt of dissolved CO2, a significant amount that could be removed from the atmosphere.

Highlights: The Serra Geral Formation basalts are suitable reservoirs for successful deployment of CO2 storage plants in Brazil, because their chemical and structural characteristics favor the carbonate mineralization, and therefore, the effective and permanent storage of CO2.

Abstract:
"In recent years, the Paris Agreement signatory countries understood the urgency for the Carbon, Capture and Storage (CCS) technologies. The CCS implementation has been growing exponentially during the last seven years, with the CarbFix (Iceland) and Wallula (USA) projects as the most successful cases. These projects focus on CO2 injection within basaltic reservoirs.
The CO2 geological storage in basalts is one of the most efficient methods in terms of injection capacity. It guarantees zero to minimal CO2 leakage due to the mineralizing reactions between the CO2-rich fluid and the Ca, Mg and Fe ions available in these reservoirs. Such reactions occur much faster compared to geological time, which results in the possibility of capturing and dissolving a greater amount of CO2 that mineralizes and precipitate in the fractures and amygdales of the basaltic formation.
Although basaltic rock formations are found both on surface and subsurface, one of the main challenges is knowing the abundance and availability of the reactive ions (Ca, Mg, Fe), since they must be found as free divalent cations for the mineralization of new carbonates. Therefore, this project intends to study the basalts of the Serra Geral Formation in the Paraná Basin, where the main Brazilian CO2-emitting industries are also located. Also, it aims to characterize the mineralogic and geochemical changes of the basalts before and after the CO2 injection. The findings will allow to determine zones with greater abundance of reactive elements and predict the favorability of carbonate mineralization to finally provide a prospect location for a CCS pilot project.
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RCGI Project number: 73

Naphthalenediimide-containing metal-organic frameworks for mixed matrix membranes designed for CO2 separation

Gabriela Oliveira, Sérgio Brochsztain, José Fernando Queiruga Rey, Caetano Rodrigues Miranda

Keywords: CO2 capture, metal-organic frameworks, naphthalenediimides

Impact: The current polymeric membranes do not guarantee adequate efficiency in CO2 separation, not having the ideal relationship between permeability and gas selectivity. Therefore, mixed matrix membranes with metallorganic networks (MOFs) have received greater attention for their improved separation efficiency, bringing applications for cleaner energy and greater sustainability.

Highlights: Mixed matrix membranes with MOFs can have the following highlights:
- cost-effective;
- higher potential for CO2 separation;
- easy operation and scalability;
- low energy costs and small environmental footprint.

Abstract:
According to the Intergovernmental Panel on Climate Change's (IPCC) sixth report of 2021, climate changes caused by human activitity are leading to more frequent and extreme weather events. These climate changes have been attributed mainly to an increase in the emissions of carbon dioxide (CO2) and other greenhouse gases (GHG). 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 or CO2/CH4 in natural gas reservoirs, 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, forming one-, two- or three-dimensional coordination networks. In the present work, we synthesized MOFs for MMMs, using 1,4,5,8-naphthalenediimides (NDIs) as the organic ligands. In 2008, the group of Joseph Hupp, from Northwestern University, Illinois, reported for the first time that a NDI-based MOF was efficient in the separation of CO2 from CH4. For that purpose, they employed N,N'-bis(4-pyridyl)-1,4,5,8-naphthalenediimide (DPNI), a NDI derivative substituted with basic pyridine ligands, and zinc as the cation. Herein, we present a novel NDI ligand, N,N'-bis(4-carboxyphenyl)-1,4,5,8-naphthalenediimide (CNDI), containing acidic carboxylic acid ligands. 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 at 120 oC, using dimethylformamide as the solvent. The MOFs were characterized by X-ray diffraction, scanning electron microscopy, UV-visible spectroscopy and N2 adsorption isotherms. The CNDI-based UiO MOF showed higher crystallinity than the material prepared with Zn. The UiO MOF also presented mesoporosity, leading to the conclusion that can be a candidate to be used in the synthesis of MMMs.

RCGI Project number: 68

Evaluation of a microbial fuel cell for the generation of electricity from thermophilic denitrification

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Keywords: Biocathode, Bioenergy e Vinasse

Impact: This project aims to investigate thermophilic bioelectrochemical denitrification using the microbial fuel cell (MFC) as a promising technology as it can simultaneously generate energy and remove pollutants from wastewater using microorganisms as biocatalysts. The focus on denitrification is in order to reduce the limitations associated with the cathode found in MFC due to oxygen reduction, because in thermophilic conditions the anode presents better electricity generation results so the system removes organic matter (anode) and nitrogen (cathode) present in the vinasse.

Highlights: Obtaining a mature inoculum with more than 400 days in operation and organic matter removal above 75%.
This project is in the prototyping stage, but we have already obtained positive sealing results, the next step is to finalize the assembly and put the reactors into operation.

Abstract:
The microbial fuel cell (MFC) is a promising technology, mainly because it has the ability to generate clean electricity from wastewater, such as vinasse. However, this technology still presents challenges and limitations for energy generation. Therefore, this project aims to use the route - autotrophic denitrification associated with the cathode to overcome the limitations of the oxygen reduction reaction under thermophilic conditions, identified by Cano et al. (2021). Four dual-chamber CCMs with continuous flow will be evaluated, three at room temperature and one at 55 °C. The experiment will have 4 operational stages Stage 1: Prototyping, Stage 2: Inoculation and adaptation, Stage 3: Coupling of the reactors and Stage 4: Effect of organic load. The analysis of the effluent treatment efficiency simulating vinasse will be evaluated by means of physicochemical and electrochemical parameters. The biofilm adhered to the anode will be collected at the end of the experiment, when DNA will be extracted and sequenced. The project is at the end of the first stage, but in parallel it is being monitored 3 inoculum reactors, INO1, INO2 and INO3 that have obtained positive results in removal of organic matter and coulombic efficiency so far. INO1 obtained removal above 75% and coulombic efficiency of 1.68%, the other 2 reactors obtained 84 and 44.6 % removal, and 1.64 and 1.07% coulombic efficiency respectively.

RCGI Project number: 56

Petrography and mineralogy of sandstones from the Rio Bonito Formation, Paraná Basin, as potential for CCS

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Keywords: Rio Bonito Formation. Sandstone. Carbon Capture and Storage

Impact:

- The sandstones characteristics understanding of the Rio Bonito Formation helps to understand the potential of these rocks for the purpose of carbon capture and storage.

Highlights:

- The sandstones of the Rio Bonito Formation have a mineralogical and textural composition favorable to CCS.
- Constituents such as feldspars (plagioclase and alkali-feldspar), carbonate (calcite), micas (muscovite and biotite), the textural framework and the diagenetic arrangement help to characterize the rock.
- The presence of clay mineral cement preserves porosity.

Abstract:
The increase in efforts to contain the effects of greenhouse gases in the atmosphere has driven the development of Carbon Capture and Storage (CCS) technologies. The geological storage of carbon in sandy units is an interesting alternative in the Brazilian scenario, where the Rio Bonito Formation in the Paraná Basin represents one of the units with great potential due to its lithology. Facies, petrographic and diagenetic analyzes in sandstones obtained in the states of São Paulo and Santa Catarina, allowed a better characterization of these rocks and their propensity to CCS. The objective of this work is to contribute with new information on the textural framework of the sandstones that constitute the Rio Bonito Formation. Nine sedimentary facies were individualized and grouped into 2 facies associations: fluvial and deltaic. The petrographic analysis individualized 3 types of sandstones: arkose, lithic arkose and subarkose. In these rocks, the main constituents are quartz grains, feldspars (plagioclase and alkali-feldspar), carbonate (calcite), micas (muscovite and biotite), clay, iron oxide-hydroxide and heavy minerals. The framework of the analyzed rocks is normal to closed, with compaction being more important than carbonate cementation for the reduction of porosity. The diagenetic stages reached were eodiagenesis (carbonate cementation, fractured grains, and presence of Fe hydroxide oxide) and mesodiagenesis (chemical compaction, feldspar dissolution features, quartz syntaxial growth, clay mineral transformation and feldspar replacement). The presence of clay mineral cement preserves porosity. Minerals such as plagioclase, alkali-feldspar and micas have a good effect on CO2 sequestration. In this way, it was observed that the rocks present heterogeneities both in terms of composition and porosity. Furthermore, the presence of clay in sandstones with wavy lamination and climbing ripples cross lamination in the delta facies association, shows a potential environment for CCS.

RCGI Project number: 58

Bioprospected Microalgae from Mangroves in a Biotechnological Perspective: The Biorefinery Concept

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Keywords: Coelastrella sp., Third-generation bioethanol, Fatty acids production.

Impact: The biomass of Coelastrella sp., a microalgae isolated from the Baixada Santista (SP) mangroves, proved to be high potential for producing third-generation bioethanol. In addition, it demonstrated the ability to accumulate fatty acids of nutraceutical interest, contributing to the biorefinery concept.

Highlights: Third-generation bioethanol is a good alternative to supply the demand for fuels, The strains bioprospecting from environments with extreme conditions proves to be a crucial biotechnological tool, Combining bioethanol production and other bioproducts with commercial interest makes the process even more attractive, Coelastrella sp. proves to be a strain of high potential within the biorefinery concept.

Abstract:

The constant increase in energy world demand, mainly related to the transportation sector, and the environmental problems associated with the exploration and use of fossil fuels, have made biofuels, like bioethanol, from renewable sources increasingly attractive. Bioethanol can be obtained from biomass like sugarcane and corn (first generation) and agricultural forestry residues (second generation). However, the competition between food versus fuel, the need for arable land use, and the use of potable water for crop maintenance have mainly driven the development of third-generation bioethanol, using microalgae as biomass. Microalgae are photosynthesizing microorganisms that, in the presence of light, CO2, and water, convert into O2 and glucose for their cellular development and maintenance. These microorganisms have fast growth, do not require potable water for their cultivation, and act directly in mitigating CO2 in the atmosphere, besides having high biotechnological potential. Under certain cultivation conditions, microalgae accumulate carbohydrates in their cells, which are easily hydrolysable for their effective fermentation and bioethanol production. However, to be successful in producing this biofuel, it is necessary to identify strains that can increase the accumulation of carbohydrates associated with high biomass productivity. Furthermore, for this procedure to be economically viable, it is necessary to associate the accumulation of carbohydrates with other bioproducts of interest, a process known as a biorefinery. Mangroves are ecosystems with unique characteristics, presenting high microbial biodiversity adapted to various pressures and, therefore, extremely attractive from a biotechnological perspective. In this work, about 40 strains were

isolated from mangroves in the Baixada Santista (SP). From these, a strain identified as Coelastrella sp. showed rapid growth and high carbohydrate accumulation, where glucose represented up to 43% of its biomass. Moreover, this strain also accumulated lipids, more expressively long-chain fatty acids (mainly C18), with emphasis on the accumulation of alpha-linolenic acid (C18:3), an essential fatty acid of the Omega 3 group, with nutraceutical application. Thus, Coelastrella sp. proves to be a potential strain considering the biorefinery concept, presenting a relevant carbohydrate accumulation for further bioethanol production, besides the co-production of bioproducts of commercial interest.

RCGI Project number: 61

Design of catalysts to hydrogenation of carbon dioxide into higher alcohols, such as ethanol, propanol and butanol.

Vinicio Simizu, Pedro Vidinha

Keywords: CO2 hydrogenation, bimetallic catalyst, supercritical CO2

Impact: One of the biggest challenges that humanity must deal with nowadays is climate change. The Earth's temperature has increased by about 2°C from the pre-industrial period (17th century) to the present day and could reach a variation of another 2°C in the upcoming years if nothing is done to reverse it. According to the US National Research Council, the accumulation of greenhouse gases (CO2 is one of them) is responsible for both the increase in atmosphere's and surface of the ocean's temperatures. Some strategies are suitable to decrease CO2 levels, like its capture and utilisation.

Highlights: The biggest challenge of all the work is choosing and tailoring catalysts that fulfill the objectives of valorisation of CO2 with both high conversion and selectivity to some of the higher alcohols, primarily ethanol. Because the stability of the molecule of CO2, the material must be suitable for thermocatalysis under high pressures and, consequently, be able to allow its hydrogenation into the desired product. Design of a bimetallic catalyst is proposed.

Abstract:

"One of the biggest challenges that humanity must deal with today is climate change. The Earth's temperature has increased by about 2°C from the pre-industrial period (17th century) to the present day and could reach a variation of another 2°C in the upcoming years if nothing is done to reverse this scenario of global warming[1]. According to the US National Research Council, the accumulation of greenhouse gases (CO2 is one of them) is responsible for both the increase in atmosphere's and surface of the ocean's temperatures [2].

Besides lowering CO¬2 emissions around the world, some other alternatives have been proposed as well, like some elegant solutions to decrease CO2 levels, which includes both its capture and utilisation[3]. In this present work, the objective is the valorisation of CO2, converting this greenhouse gas into products of interest to the industry, also known as high-value products. The main desired outcome are higher alcohols (ethanol, 2-propanol, propanol and butanol, for example), however molecule such as methanol is also acceptable.

The biggest challenge of all the work is choosing and tailoring catalysts that fulfill the objectives of valorisation of CO2 with both high conversion and selectivity to some of the higher alcohols, primarily ethanol. Because the stability of the molecule of CO2, the material must be suitable for thermocatalysis under high pressures and, consequently, be able to allow its hydrogenation into the desired product[4].

Primarily, the catalyst was thought to work over two steps, which the first one is responsible for the CO2 hydrogenation into carbon monoxide, process also known as Reverse Water Gas Shift (RWGS), and the second step should be able to reduce carbon monoxide into ethanol. Therefore, a bimetallic catalyst was designed to attend these two necessities, where first metal is suitable for carbon monoxide production, as palladium (Pd), and the other is well known by C-C coupling in Fischer-Tropsch reactions, as iron (Fe) and cobalt (Co)[5,6,7]. Combining both metals over a good support for CO2 hydrogenation into methanol, as TiO2, this material should be an applicable catalyst to produce ethanol and other higher alcohols[8].

Until the present date, mono and bimetallic catalysts were synthesized under different conditions to validate the previous thesis, such as Pd/TiO2, Pd-Fe/TiO2 and Pd-Co/TiO2. They were tested and

proved that these combinations can affect positively the development CO2 into high-value products, shifting them from carbon monoxide (for Pd/TiO2) to methanol, ethanol, and propanol. Also, the bimetallic catalysts were able to improve the conversion of the reaction, jumping from 8 to 20% in a batch reactor.

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RCGI Project number: 63

Succinic acid production by Bacillus spp. under supercritical CO2

Maria Luisa Zardo, José Gregorio Cabrera Gomez, Pedro Miguel Vidinha Gomes

Keywords: Succinic Acid, Supercritical CO2, Bacillus

Impact: Chemical compounds are predominantly produced through catalytic processes from non-renewable sources. The replacement of these routes by biosynthetic pathways makes the cost of production lower and eco-friendly. Increasing the availability of CO2 through its supercritical fluid can improve the production of succinic acid by microorganisms, transforming C1 compound into C4.

Highlights: We present a collection of 56 strains of Bacillus spp. able to survive and grow in supercritical conditions of CO2. All strains are being analyzed for the presence of by-products with high added value. Specifically strain C2.31 was able to produce a relevant amount of succinic acid and can go through metabolic engineering strategies to obtain an efficient bioprocess under sCO2.

Abstract:
Succinic acid (SA) was considered one of the top 10 building blocks of chemical industry with great potential to be produced by biosynthetic pathways. Their applicability is diverse, can be used as manufacture to synthetic resins or as intermediary of derivatives such as gamma-butyrolactone, 1,4-butanediol and tetrahydrofuran. The traditional SA production is derived from catalytic processes of non-renewable sources and suffers from environmental pollution. Nowadays, 7 biological pathways were described as natural or engineered SA producers. The most explored is the reductive branch of tricarboxylic acid cycle coupled with carboxylases, which converts PEP/pyruvate into oxaloacetate (OAA). This important step can assimilate 1 mol of CO2 to each form OAA, fixing carbon in the process. The supercritical CO2 (sCO2, 31,1°C, 73 bar) could be an interesting strategy to improve the diffusivity of this molecule on the broth media, increasing the SA production, avoiding cross-contamination due high pressure and at same time being attractive for their price and low toxicity. Most bacteria from genus Bacillus are aerobic or facultatively anaerobic, chemoorganotrophic, gram-positive rods, which can be cultivated on a wide range of pH and temperature, forming resistant endospores. The goal of this work is to identify strains of Bacillus spp. that produce SA under sCO2 conditions. A germplasm bank of Bacillus spp. with 200 strains isolated from the Brazilian Cerrado was kindly provided by collaborators. Each strain was cultivated in LB medium for morphological characterization and cell multiplication. A consortium including all strains was inoculated in modified M9 medium (microaerophilic, 20-60 bar, 35°C, with agitation) for 21 days. To isolate individual SA producers, reactors containing the highest cell concentrations were passed into fresh culture medium for 2 subsequent rounds of incubation at the same conditions, except by pressure at 100 bar. A total of 56 strains were isolated and cultured in mineral medium, supplemented with glucose and ammonium sulfate (microaerophilic, 1 bar, 35°C, 48h, 150 rpm). Among these, strain C2.31 showed the highest production of SA (0,8 g/L) and a co-production of organic acids, representing a good starting point to improve the biosynthetic pathway and metabolic engineering of succinate production under supercritical CO2.

RCGI Project number: 63

Synthesis of MWW and hierarchical lamellar zeolites by mechanical treatment for application in the Methanol to Olefins (MTO) reaction

Diego Sarmento Duncan Lima, Laura Lorena Silva, Leandro Martins

Keywords: Methanol-to-olefins, ITQ-2, Ball-milling

Impact: Development of a new low cost, efficient and practical mechanical method for the synthesis of hierarchical and delaminated zeolite, similar to ITQ-2. Development of a catalyst more resistant to deactivation by coke and with favorable application in the methanol to olefins reaction.

Highlights: The industrial process Methanol to olefins is a promising alternative technology for the production of olefins without dependence on fossil reserves. However, this process is limited by the deactivation of the catalysts by coke. ITQ-2 zeolite has a structure that is more resistant to this deactivation process. The ball-milling method was applied to the synthesis of a zeolite analogous to ITQ-2, which demonstrated high efficiency, practicality and low cost.

Abstract:
The methanol-to-olefins (MTO) industrial process has proved an important strategy for the production of chemical commodities, such as ethylene and propylene, while reducing dependence on fossil reserves and CO2 emissions. In search of the optimization of this catalytic process, much has been investigated about new zeolitic structures that are more resistant to deactivation by coke, the main limiting factor of MTO. In view of this, the lamellar catalyst ITQ-2 is a strong candidate for application in the process due to its hierarchical character arising from the disorganized state of its layers. However, the high cost and low yield of the preparation of this material limits its industrial applications. In view of this, the current work aimed to prepare a catalyst analogous to ITQ-2 through a faster, economically viable and efficient mechanical treatment, the ball-milling. For the preparation of the hierarchical catalysts, the precursor zeolite, MCM-22(P), still wet, were conducted to two different treatments: chemical and mechanical. This first refers to the conventional method of synthesis of ITQ-2, which the precursor material undergoes an swelling and delamination process through the addition of chemical agents such as hexadecyltrimethylammonium bromide (CTABr) and alkylammonium hydroxide (TPAOH), and subsequent sonication and acid treatment. While the mechanical treatment consists of the application of MCM-22(P) in the vibrating ball mill using a vibration frequency of 25 Hz for 30 minutes. The mechanically and chemically delaminated materials were characterized by X-ray diffractometry (XRD), nitrogen physisorption, scanning and transmission electron microscopy (SEM and TEM) and temperature programmed pyridine desorption accompanied by FTIR (TPD-Py). XRD results indicated a long-distance loss of ordering of the treated materials in view of the lamellar disorganization, while the images obtained by SEM and TEM confirm and emphasize the random state of the layers. The nitrogen physisorption isotherms show the reach of the hierarchical state of both materials due to the presence of meso and micropores. On the other hand, the TPD-Py results show that the mechanically delaminated material had a higher number of acid sites compared to the conventionally treated material, 472 and 175 Py µmol/g, respectively. This difference is due to the greater accessibility to acidic sites of the mechanically delaminated material and also the conservation of sites, that are commonly lost during chemical treatment. Through the results obtained, it was evidenced that the mechanical treatment has advantages over the chemical treatment due to its simplicity, low cost, and preparation of a more active catalyst. In addition, the promising application of the delaminated material in the MTO reaction is highlighted.

RCGI Project number: 63

Optimization of a thermophilic microbial fuel cell with optimized external resistance

Julio Cano (University of Sao Paulo), Vitor Cano (University of Sao Paulo) Marcelo Antunes Nolasco (University of Sao Paulo)

Keywords: Microbial fuel cell, optimization, bioelectrochemical system, bioenergy, electricity.

Impact: Electric energy is essential for human well-being, for social and economic development. In turn, the use of energy from fossil gases has several problems associated with the emission of the greenhouse effect. According to the Intergovernmental Panel on Climate Change, 42 Gt of carbon dioxide from use are released annually. Fossil fuel deposits are limited alternatives as far as they are efficient, as there are millions of formation for these compounds. Not least, the speed of fossil extraction and consumption makes the same impossible, a finite resource, a finite resource In addition to advancing the energy transition, renewable energy sources become dominant in the exercises to make decarbonization the economy is increasingly targeted. Therefore, it is necessary to progressively diversify the means of energy production and the transition to a carbon economy with greater use of alternative, clean and renewable sources Vinasse, as a sub-production of ethanol, has great energy potential, as it presents A composition with high concentration of nutrients Thus, in natura vinasse is commonly used for fertigation, which despite the benefits generated by fertilization when produced for long periods can cause salization in natura and imbalance of soil nutrients. Thus, in addition to the environmental impacts of energy issues, industrial development and population problems contribute to the increase in wastewater in nature with a high polluting load, eutrophication and the spread of diseases. Combining the need for electricity with new forms of energy generation, such as energy treatment plants, treatment plants become potential producers of electricity. fuel, since it can generate water resources, since water resources, water treatment, can generate electricity, a water resources treatment, since water resources, since water resources can be used to contribute. Currently, an optimization of the CCMs, configuration, choice of materials, or by the reactor community is sought for the development of bacteria plus one for the removal of organic matter and energy generation.

Highlights:

A novel compact MFC design optimized utilization of low-cost electrodes.

External resistance influenced balance between conversion efficiency and power.

Optimization of operation operating conditions has been beneficial for an internal resistance repair of the anodic chamber, main for thermophilic reactors.

Abstract:
The development of new technologies to supply the energy demand and for the management of wastewater treatment becomes increasingly relevant. With this in mind, the microbial fuel cell (MFC) presents itself as a promising technology to be used in wastewater treatment. Besides being a technology that allows the direct conversion of organic matter into energy electricity from different substrates, including wastewater. However, there are still technical and process limitations to improve the technology, aiming at greater efficiency. In this way, this project aims to analyze the effect of the temperature rise together with the optimization of the external resistance for the parameters of energy generation, removal of organic matter. The study was carried out with a bench-scale tubular MCC, applied to the treatment of synthetic effluent simulating vinasse. Six MCCs (R1, R2, R3, R4) were

operated under continuous flow, studied in 3 conditions/phases, all with a value of 5 gCOD/L. Phase 1 for standardization of all units, phase 2 with alteration of Rext (22.5Ω) in reactors at room temperature (R1 and R2) and at 55ºC (R3 and R4). The analysis of the effluent treatment efficiency is being evaluated through the analysis of physical-chemical and electrochemical parameters. To determine the internal resistance, the polarization curve and the electrochemical impedance spectroscopy technique are used. To determine the internal resistance, the polarization curve and the electrochemical impedance spectroscopy technique are used. The first phase of operation has already made it possible to obtain data indicating that the units R1, R2, R3 and R4 were considered as replicas, with total potential above 600 mV, removal of organic matter above 70% and internal resistance below 13 Ω. The second phase demonstrated that the strategy adopted for the atomization of the anodic chamber was superior to the first phase of operation. The resistance optimization allowed the increase of the current that presented average values of 14 mA for the thermophilic reactors, 10 mA for the mesophilic reactors. This made it possible for thermophilic units with optimized external resistance to present 14% coumlombic efficiency. Thus, the operational strategy for anodic optimization was efficient, for operation at 55°C with external resistance of 22.5 Ω. Thus, through an interdisciplinary approach, this study contributed to the development of a technology for clean energy generation.

RCGI Project number: 65

Carbon Nanotubes for CO2/N2 Separation: Insights from Grand Canonical Monte Carlo Simulations

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Keywords: Gas separation, Monte Carlo Simulations, Membrane technologies

Impact: Carbon nanotubes (CNTs) are known to improve the mechanical properties of membranes when embedded in a polymeric matrix. This research explores the selectivity of carbon nanotubes for N2/CO2 separation. Our results show that carbon nanotubes have high selectivity of N2 over CO2, suggesting that their incorporation into membranes might also enhance their separation properties.

Highlights: Carbon nanotubes present high selectivity for N2 over CO2 in an ambient similar to flue gas
Simulations indicate that carbon nanotubes present selectivity from 2.9 to 100%

Abstract:
"Due to the emerging need to reduce carbon emissions, a great effort has been made to efficiently separate carbon dioxide (CO2) from nitrogen gas (N2), the main component of flue gas. However, this separation is challenging because these molecules have similar kinetic diameters [1]. A class of promising materials for gas separation is carbon nanotubes (CNTs), due to their outstanding mechanical properties and good chemical stability. Under certain conditions, it is possible to incorporate CNTs into a polymeric membrane to improve its mechanical properties. Furthermore, these nanostructured materials might be used to select molecules by exploring confinement effects, since it is possible to synthesize CNTs with diameters similar to the diameter of small molecules (~10 Å). In this study, we perform a series of Grand Canonical Monte Carlo simulations, within the Cassandra software, at 315.30 K and 1 atm to evaluate armchair and zigzag CNTs with different diameters, from 10.84 to 16.27 Å for N2/CO2 separation. The interactions between the gas molecules and the nanotubes were described through novel force fields tunned by first principles calculations and developed to explore the use of carbon nanomaterials for N2/CO2 separation. The results show that the selectivity of CNTs under similar conditions to flue gas (85 % of N2 and 15% of CO2) depends on their diameter and chirality. The obtained selectivities vary from 2.9 to 100% in favour of N2 over CO2. The mechanism behind the high selectivity might be the difference in van der Waals radius of N2 and CO2. Since the molecules are in a confined environment, the CNT may favour the species with the smallest radius, which is N2. These results suggest that carbon nanotubes are promising materials for N2/CO2 separation, and their incorporation in membranes might lead to enhanced selectivity towards N2.

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Brazilian Policies and Legislation for greenhouse gases

Cardoso, M., Deliberari, L. R., Costa, H. K. M., Sousa, A., Barbosa, Araújo, I. L., Motta, K. K. M., Moutinho dos Santos, E., Mouette, D.

Keywords: GHG emissions, industry, sustainability

Impact: The risk offered by warming caused by emission of Greenhouse Gases (GHG), especially CO2 and CH4, which are the main characters for reductionist and conservationist policies aimed at sustainability and sustainable development. Andrade and Mattei (2013) highlight the increasing dependence on fossil fuels which points are important for discussions about energy transition.

Highlights: About 60% of greenhouse gas emissions come from just ten countries, while other 100 countries emit less than 3% of it. The industrial sector accounts for about 30% of global GHG emissions, this is equivalent to the share of global energy use. The majority of industrial emissions-typically between 60-80% depend on definitions - originate from energy -intensive primary materials in the EIIs production (Fischedick et al., 2014).

Abstract:
"Among the responses from Paris Agreement about global warming and GHG emissions reduction, the Nationally Determined Contributions (NDC), a voluntary commitment to GHG emissions reduce and adapt to the impacts of climate change established among signatory countries that allow each country to adapt its actions, defining laws and public policies for decarbonization in different segments of the economy - including land use, transportation, industry, and energy - according to their reality, needs and available resources. The general character of the NDCs revolves around the theme of GHG emissions control and adaptation to the effects of climate change. The Brazilian environmental agenda is regulated by the Ministry of Environment (MMA), and the Brazilian NDC reaffirms the commitment to reduce total net GHG emissions by 37% in 2025, officially commits to reduce Brazilian emissions by 43% by 2030 and enunciates the indicative goal of achieving climate neutrality - that is, net zero emissions - in 2060 (IBTS, 2020).
Industrial emissions have continued to grow since 1990, despite the global climate policy framework. The demand for basic materials produced by electro-intensive industries has also increased over the decades. Most materials are traded in commodity markets based on standard products, high volumes, and price competition. (Åhman, et al., 2017). Therefore, current economic models associated with growing needs for basic materials make the industrial sector essential to GHG neutralization goals.
For this reason this article assesses existing policies focused on manufacturing sector to mitigate GHG emissions. In addition, it intends to understand the mechanisms and solutions of those who were successful in their purpose and, finally, to understand the gaps that still need to be filled.
Greenhouse gases absorb heat and release it gradually over time, like bricks in a fireplace after a fire goes out. Without this reaction, the Earth's average annual temperature would be below freezing. However, the increase in greenhouse gases caused by human actions has caused an energy imbalance on Earth, trapping additional heat, and raising the planet's average temperature (NOAA, 2021).
These effects are sufficient to affect humanity, economic activities, and the environment. In recent decades, there has been a rise in the ordinary sense of local and world population. About of the environmental topic, there are need for recovery, mitigation, and a paradigm shift to control the consequences for the development and flow of human activities. We can also observe efforts and discussions in the direction of control, legislation, and regulation of human activities for the least possible impact on the already overloaded environment.
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RCGI Project number: 69

Bioenergy's Social Perception and Its Relevance to Energy Transition

Giovana Turquetti, Karen Mascarenhas, Sigmar Malvezzi

Keywords: bioenergy, social perception, energy transition

Impact: It is common knowledge that energy transition is central to climate change action. One of COP26's main objectives is to mobilize countries and reach ambitious emissions reduction targets by 2030 that align with reaching net zero by the middle of the century. Within this context, bioenergy is one of the leading low-carbon solutions for the future, considering its versatility and biomass low carbon footprint. However, the installation and success of energy projects do not depend exclusively on industry plans as social perception interferes in its acceptance. When it comes to residents who live close to bioenergy projects, their opinion and impressions are fundamental to the project's continuity. For this matter, understanding how social perception works and the factors that influence the way people perceive energy transition is essential.

Highlights: Bioenergy is a crucial low-carbon solution for climate change action. Using a variety of biomass sources, different products or energy services are obtained from bioenergy production such as ethanol, biogas or thermal energy.
Research indicates that some of the main negative perceptions on bioenergy include land-use changes linked to biofuel production and social concern over food-crops competitions.
The public seems positive about second-generation fuels when informed about them.
The Social Acceptance theory (Wüstenhagen et al., 2007) is one of the most applied theories in social perception on bioenergy papers to explore and understand how acceptance works.

Abstract:
Bioenergy is a sustainable alternative for energy production, standing out for its versatility in raw materials and forms of use. Its production occurs through the conversion of biomass - organic matter of plant origin - into energy, presenting itself as a substitute energy source for fossil fuels as it comes close to having carbon neutrality. 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. In this study, we analysed 103 papers selected in Scopus that had public or social perception or acceptance of bioenergy as their subject aiming at the investigation of the main impact factors and theories studied in this area. The findings point out that the resistance against bioenergy in ethanol production derives from the land use competition between crops for fuel or food and the change in the landscape. 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, it is fundamental to research and interpret the public's perception of bioenergy using Social Sciences such as Social Psychology for an in-depth comprehension of society's views and sentiments related to bioenergy and use this knowledge to facilitate dialogue and engagement towards the carbon neutrality agenda.

RCGI Project number: 70

Scaling-up Strategies for Battery-like Electrodes Deployed for Direct Lithium Extraction from Geothermal Sources

Victor Sumikawa, Andressa Mota-Lima, Claudio Augusto Oller do Nascimento*

Keywords: Lithium-battery, Electrochemistry, Scale-up

Impact: Scalling-up a baterry-based electrode is non-trivial task that requests well defined strategies for a reliable acomplishiment.

Highlights:
1- Battery-like electrodes enable a more effective and selective lithium recovery,
2- Electrochemical pumping technology,
3- Challanges of Scaling-up,
4- Electrode surface side-reaction and the Oxygen Evolution Reaction (OER),
5- Geometry restrictions and the electrical conductivity,

Abstract:
"The worldwide quest for lithium to supply the continuously fast-paced demands driven by the automotive lithium-battery market has steered the search for technologies that enables a more effective lithium recovery. In this context, the use of battery-based electrodes in the so-called electrochemical pumping technology gained attention because it simplifies the whole process the most. Recently, a pilot scale cell prototype was constructed, and the concept of recovering pure lithium from brine was proved (Palagonia et al., 2020). In the work of Professor Fabio La Mantia, it was used ultrapure water with 120mM of KCl as the initial recovery solution, which enables the recovery of 100mM LiCl plus 1mM KCl after the treatment.

In this present work, we move the challenge up, we engage with the scaling-up task. We used the proof-of-concept pilot cell of Professor Fabio La Mantia's group as a model cell. The aim is to increase the area of this model cell by over two hundred times. For that, a vertical column containing 10 cm in diameter, see Figure 1, is going to be used as the support for piling up several layers of electrodes.

We foresee the following issues regarding the scaled-up battery-like electrode set:

1 – Exit of the oxygen bubbles formed on the electrode surface due to the side-reaction, which can be safely attributed to the Oxygen Evolution Reaction (OER). The increase of the bubble size degrades the performance of the technology because it decreases the effective area of the brine-oxide interface. According to Calvo and co-workers (Marchini et al., 2018, Romero et al., 2021), lithium capture supports 85% of the electrical current that crosses the electrode, meaning that the other 15% is channelled by OER. Based on this information, the mole ratio of 1 O2 to 17 Li+ is expected.

2 – The flow through geometry imposes a constriction on the maximum area each electrode foil can have, mostly because of the electrical conductivity of the carbon support (carbon cloth).

In the post section of the ETRI meeting, the audience can learn about the strategies we will employ to enable a reliable scaling up.

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Stability of water nanodroplets: modeling atmospheric phenomena at nanoscale by molecular dynamics

Jacqueline Teixeira Santos and Caetano Rodrigues Miranda

Keywords: nanodroplets, aerosol, molecular dynamics

Impact: Aerosols contribute to global cooling by counterbalancing the warming caused by CO2 emissions. Due to these contributions, aerosols are still indispensable for the climate model.
However, aerosols have a very large variety of particles which makes their characterization difficult. In this way, we seek to understand the entropy aspects of a supercooled nanodrop in the atmosphere from a molecular point of view.

Highlights:

The results showed that the nanodrop radius equal to 1nm becomes unstable, breaks, and forms clusters in the presence of a concentration of 4 molecules of NaCl.

Abstract:
Aerosols contribute to global cooling by counterbalancing the warming caused by CO2 emissions. However, the formation of water droplets and the salt effect have not been fully understood. Here, it was studied in a nanodrop model that describes atmospheric aerosols through molecular dynamics simulations with the LAMMPS package. We used the force field TIP4P/2005 for the water model with an initial temperature of 20K to 273K in the equilibration phase. The stability of these nano drops was investigate over the concentration of NaCl salts as a function of volume. Understanding this system's stability will be important for future studies involving water droplets in the presence of sulfates. There is a particular interest in obtaining the preferential region where the ions are located regarding the droplet radius, salinity, and temperature. We start with a sphere of 1 nm radius for different salt concentrations, ranging from 1 to 4 molecules of NaCl, with a fixed amount of water molecules (380 molecules). We focused on the study of the stability of a nanodrop in a vacuum with different ion concentrations and nanodroplet diameters. The results showed that the nanodrop radius equal to 1nm becomes unstable, breaks, and forms clusters in the presence of a concentration of 4 molecules of NaCl.

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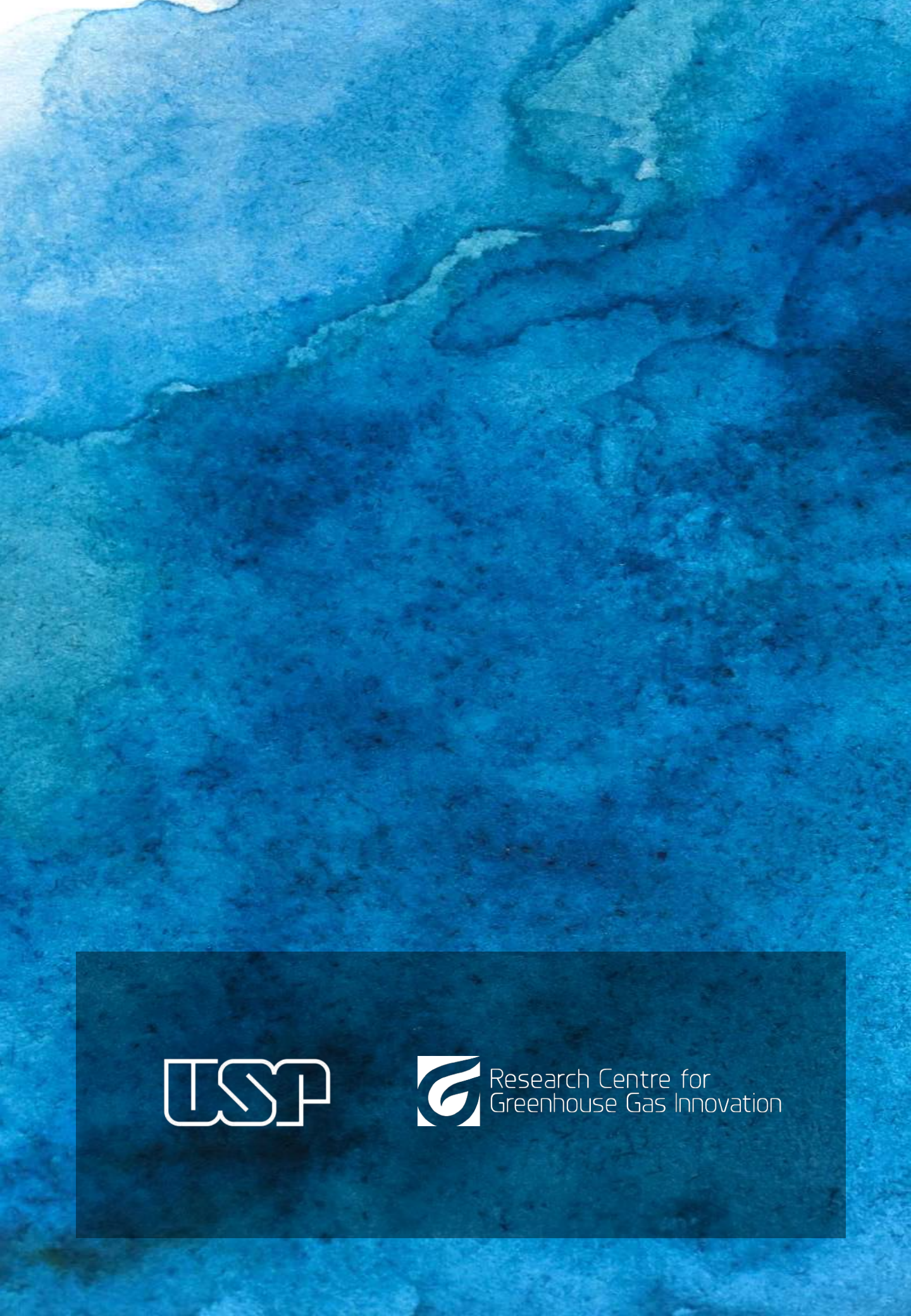
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