Energy Transition

RESEARCH & INNOVATION

SÃO PAULO, BRAZIL - 2019

BOOK OF ABSTRACTS

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Energy Transition Research & Innovation

The RCGI – Research Centre for Gas Innovation is proud to host its fourth annual conference in Brazil. ETRI 2019 – Energy Transition Research & Innovation brings together companies, government, funding agencies and academia to discuss technological advancement and develop joint mechanisms for research and innovation in the field of energy transition.

A two-day event at the University of São Paulo, ETRI 2019 attendees will learn from CCS (carbon capture and storage) projects worldwide and discuss goals and initiatives to support the CCS roll-out towards zero emissions. More than 120 presentations will showcase the key results of RCGI projects, followed by constructive discussions from two panels of specialists.

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Cleaner energy for a sustainable future

Founded by FAPESP and Shell at the University of São Paulo, Brazil, the RCGI – Research Centre for Gas Innovation is the result of a partnership in support of high-level scientific research for the development of the energy sector.

With our activities based on three pillars: research, innovation and diffusion of knowledge, we bring together a team of more than 350 researchers from various fields of science and technology concerned with sustainable development in a worldwide energy-transition scenario.

By integrating 46 projects into 5 research programmes, we contribute offering innovative solutions to the technological problems related to natural gas, biogas, hydrogen, storage and usage of CO2 as well as providing support for the improvement of energy policies in Brazil and worldwide.

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ETRI 2019

ENERGY TRANSITION RESEARCH AND INNOVATION
UNIVERSITY OF SÃO PAULO, BRAZIL
1-2 OCTOBER 2019

BOOK OF ABSTRACTS

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Research Centre
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GENERAL PROGRAMME: TUESDAY, 1 OCTOBER 2019

	08:00	**Registration and welcome coffee**		
OPENING CEREMONY	09:00	**Opening ceremony**		
		Prof. Gustavo Assi, *ETRI Chairman*	RCGI Director for Diffusion of Knowledge, University of São Paulo	
		Prof. Julio Meneghini	RCGI Scientific Director, University of São Paulo	
		Mr. David Torres	Vice President of Integrated Gas and CO2 Abatement Tech. at Shell Global Solutions	
		Mr. Alex Garcia de Almeida	ANP Brazilian National Agency of Petroleum, Natural Gas and Biofuels	
		Mr. Marcos Penido	São Paulo Secreatry for Infrastructure and the Environment	
		Prof. Marco Antonio Zago	President of FAPESP - São Paulo Research Foundation	
		Prof. Sylvio Canuto	Provost for Research, University of São Paulo	
KEYNOTE TALKS	09:45	**Owen Anderson -** University of Texas at Austin, USA		
		Are you a climate-change alarmist, skeptic, or fatalist? Can CCCS be a partial answer to our climate change challenge?		
	10:20	**Alex Garcia de Almeida -** Brazilian National Agency of Petroleum, Natural Gas and Biofuels		
		The role of the Regulator in energy-transition operations in Brazil		
TECHNICAL SESSIONS	11:00	**Poster session P** (with coffee break)		
		Posters P.01 to P.18. Choose two presentations to follow from the POSTER PROGRAMME.		
	11:40	**Parallel session A.1 (room 1)**	**Parallel session A.2 (room 2)**	**Parallel session A.3 (room3)**
		Leakage and monitoring	*Transport phenomena*	*Market and modeling*
		Choose your presentations from the PARALLEL SESSIONS PROGRAMME.		
	13:00	**LUNCH BREAK**		
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		Making the Future – Open Innovation at Shell		
	15:15	**Eric Larson** - Princeton University		
		The Rapid Switch project, and some thoughts on CCS in energy transitions		
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		Transportation	*Fuel cells*	*Policies and Regulation 1*
		Choose your presentations from the PARALLEL SESSIONS PROGRAMME.		
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		Posters Q.01 to Q.18. Choose two presentations to follow from the POSTER PROGRAMME.		
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		Panelists	Lene Hviid	
		Paulo Artaxo (moderator)	Eric Larson	
			Owen Anderson	
			Julio Meneghini	
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GENERAL PROGRAMME: WEDNESDAY, 2 OCTOBER 2019

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	09:55	**Alissa Park** - Columbia University, USA *Towards Sustainable Energy and Materials: Carbon Capture, Utilization and Storage*		
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		Choose your presentations from the PARALLEL SESSIONS PROGRAMME.		
	12:30	**LUNCH BREAK**		
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	14:45	**Adam Hawkes** - Imperial College London, UK *CCS in the UK: 3rd time lucky?*		
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		Choose your presentations from the PARALLEL SESSIONS PROGRAMME.		
	16:50	**Poster session S** (with coffee break) Posters S.01 to S.18. Choose two presentations to follow from the POSTER PROGRAMME.		
PANEL	17:30	**Panel: *CCS urgent actions: How, Who and When?***		
		Panelists Paulo Artaxo (moderator)	Alissa Park Adam Hawkes Chinnakonda Gopinath Rob Littel	
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PARALLEL SESSIONS PROGRAMME - 1 OCTOBER 2019

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	A.1.2	Guilherme de Sá Valadão Lopes	Monitoring Gas Leakages in CCS Operations - Passive Acoustic Monitoring of Underwater Bubble Plumes
	A.1.3	Paulo Hubert	Deep learning architectures for underwater leakage detection
	A.1.4	Eduardo Landulfo	IMPLEMENTATION OF CH4 (METHANE) RAMAN LIDAR DETECTION SYSTEM FROM ANTHROPIC SOURCES
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	A.2.2	Carlos Massaiti Okubo Júnior	Centrifugal Impeller Design using the Topology Optimization Method
	A.2.3	Elóy Esteves Gasparin	Sensitivity Analysis of the blade angles and thicknesses of an Air Centrifugal Compressor Impeller
	A.2.4	Ali Allahyarzadeh Bidgoli	Thermodynamic analysis of multi-stage compression system for CO2 injection
Market and Modeling	**A.3.1**	Oswaldo Luiz do Valle Costa	A Multiperiod Peak Period Model for Electricity Planning in Brazil Under CO2 Emission Constraints
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	A.3.3	Suani T Coelho	Biogas and biomethane potential for municipalities in Sao Paulo State
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	C.3.4	Karen Mascarenhas	Innovative Actions of the Research Centre for Gas Innovation building the path towards Sustainability Goals in Brazil
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P.04	Helio Villanueva	Development of a natural gas burner using the flameless oxidation concept
P.05	Guenther Carlos Krieger Filho	Numerical analysis of differential diffusion effects and determination of flammability limits in methane oxy-fuel combustion using detailed chemistry
P.06	Ananda Vallezi Paladino Lino	Methane tri-reforming: gas hourly space velocity and feed composition studies over Ni/CeZrO2/MgAl2O4 catalyst
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POSTER PROGRAMME - 2 OCTOBER 2019

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ABSTRACTS OF PARALLEL SESSIONS

Parallel session topic: *Leakage and Monitoring* **# A.1.1**

LABYRINTH SEAL DESIGN USING TOPOLOGY OPTIMIZATION METHOD

Bruno Caldas, Shahin Ranjbarzadeh, Renato Picelli, Emilio Carlos Nelli Silva
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Keywords
Topology Optimization, Labyrinth Seal, Finite Element

Impact statement
Uncontrolled CO2 emissions can have a significant influence on climate impacts. The reduction of emission occurs in wet and dry seals in compressors and turbines has a key role in total CO2 emission reduction. The studies show that significant emission sources are related to pneumatic devices/pumps and equipment leaks, accounting for approximately 60% of CO2 emissions.

Highlights
in this work, we present the formulation of the Topology optimization method based on 2D axisymmetric swirl flow model for designing the labyrinth seals with focus on emission reduction of fluid passes through. Then we investigated a topology optimization method on fluid-structure interaction in Labyrinth Seal.

Abstract
Uncontrolled CO2 and CH4 emissions can have a great influence on climate impacts. Studies show that the major emission sources are related to pneumatic devices/pumps and equipment leaks, accounting for approximately 60% of emissions. In the quest to reduce the climate effects caused by CO2 and CH4 emissions, the improvement of the labyrinth seals in multi-stage pumps, and compressors becomes a necessity. The concept of labyrinth seals is essentially a series of extended surfaces forming chambers between an axis and a fixed bearing, which causes turbulence in the fluid which inhibits its leakage. For many years, improving the design and performance of labyrinth seals has been a challenge in engineering. Considering the very high number of geometrical parameters in labyrinth seals and the difficulty related to determining their impact on leakage, the topology optimization is a possible approach to achieve less leakage. Thus, in this work, we present the formulation of the Topology optimization method based on 2D swirl flow model for designing the labyrinth seals with focus on emission reduction of fluid passes through. The two-dimensional and two-dimensional swirl mathematical formulation is implemented, and the optimization problem is solved by using Sparse nonlinear OPTimizer (SNOPT) solver. The objective function adopted in the labyrinth seals topology optimization is the minimization of the dissipation energy. Computational fluid dynamic (CFD) calculation is based on laminar flow. The topology optimization results demonstrate a significant reduction in fluid leakage compares to the traditional one. This project investigates the possibility of Ionic Polymer Metal Composites (IPMC) integrated labyrinth seals. The interaction of the IPMC with flow inside the labyrinth seals absorb their energy and release at the appropriate phase. In the last part of the project, a Topology Optimization Method consists of density method, fluid domain introduced by Borvall, Solid Isotropic Material with Penalization and solver by using Topology Optimization of Binary Structure (TOBS) method is developed and coupled with chemo-electro-mechanical model and Navier-Stokes equations to obtain the the topology optimized geometry of the IPMC integrated labyrinth seals (IPMC-fluid Interaction) and optimize the performance of the labyrinth seals.

Parallel session topic: *Leakage and Monitoring* **# A.1.2**

Monitoring Gas Leakages in CCS Operations - Passive Acoustic Monitoring of Underwater Bubble Plumes

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Paulo Hubert, Linilson Rodrigues Padovese
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Keywords
CCS; Leakage Monitoring; Acoustics

Impact statement
European Directive states that CCS reservoirs monitoring plan should be established. In the occurrence of leakages. Directive 2003/87/EC requires the surrender of emissions trading allowances for any leaked emissions. Therefore, the early detection of leakages will not only avoid environmental impacts but will also avoid economical impacts on CCS operations and storage permits withdrawal.

Highlights
Simulated leakages by controlled gas release experiments. Assessment of hydrophones detection ranges. Leakage detection methodologies. Leakage detection techniques in noisy environments.

Abstract
One of the challenges in Carbon Capture and Storage (CCS) is guaranteeing minimum leakage conditions in the reservoir. Some researches indicate that even small leakage would impose a severe economic risk on the operation and harsh environmental damages. Therefore, monitoring the occurrence of leakages in CCS is needed to achieve the proposed atmospheric GHG reduction. In order to assess the impacts associated with leakages, controlled gas release experiments were performed in the recent past, and in some cases, those experiments also aimed leakage detection capabilities. For underwater CCS operations, the use of passive acoustic monitoring is proposed for the detection of gaseous leakages. However, the development of passive acoustic leakage detection methodologies is a challenge as the amount of information available is still minimum. Aiming at this gap, our group planned and performed controlled leakage tests in several environments for different leakage conditions and distances between leakage sources and sensors. This presentation will first describe the sound emitted by the bubble plumes formed from underwater leakages, we will discuss how the environmental conditions, leakage composition, and exhaust geometry will affect the signal emitted by bubble formation. Then we will talk about the experiments performed by our team, and discuss the techniques we are using to detect underwater gas leakages in both silent and noisy environments.

Deep learning architectures for underwater leakage detection

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Keywords
ccs;leakage;deep learning

Impact statement
CCS underwater geological structures are candidates to store greenhouse gases; however, these structures are subject to gas percolation, leading to leakages. Project 33 of the RCGI initative is concerned on designing leakage detectors using Passive Acoustic Monitoring. This work studies the use of deep learning algorithms in the design of detectors

Highlights
CCS using deep sea geological structures are subject to leakage Passive Acoustic Monitoring is a cheap and effective way to monitor these facilities Experimental data has been obtained in various conditions Use these data to learn a precise characterization of the signal Deep Learning can be applied to learn this characterization

Abstract
CCS projects are receiving a lot of attention in the past few years. One recent idea is to use deep sea geological structures to store greenhouse gases. In these structures, however, the stored gas might percolate its way out, eventually leaking back to the atmosphere. Project 33 of the RCGI is concerned with the use of Passive Acoustic Monitoring to detect these leakages. From the past months, we have been conducting many experiments in various conditions, building a rich data set of simulated leakages and their acoustic emissions. Our goal is to use these data to obtain a precise characterization of the signal of interest. This characterization can then support the design of efficient detectors that are likely to work well in the actual operational setting of a CCS. In this work we investigate the application of Deep Learning architectures, specially Convolutional Neural Networks and Recurrent Neural Networks, to this setting. We use deep networks to learn patterns from the simulated leakages in our experimental data, and analyze the possibility of applying these learned models to signals generated in different background conditions.

Parallel session topic: *Leakage and Monitoring* **# A.1.4**

IMPLEMENTATION OF CH4 (METHANE) RAMAN LIDAR DETECTION SYSTEM FROM ANTHROPIC SOURCES

Eduardo Landulfo*, Fernanda M. Macedo*, Thais Correa*, Elaine Araujo*, Izabel Andrade*, Antônio G. Arleques*, Juliana Tavares de Melo Miranda*, Jonatan da Silva*, Roberto Guardani**
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Keywords
CH4, LidarRaman, Remote Sensing, Biomass Burning, Green House Gases

Impact statement
Innovative technology that studies the presence of various compounds of interest, like fugitive emissions, allowing further development in the study of pollutants dispersion and interactions between different chemical species under different climatic conditions.

Highlights
Methane remote sensing monitoring.
System that will assist and identiying methane sources.
The Raman technique provides the development of a less complex and lower value-added system.
The use of CRDS for CH4 primary characterization in the metropolitan region of São Paulo was enriching, guiding the acquisitions and supporting its quantification.

Abstract
Fugitive emissions, defined as unintended or irregular leaks of gases and vapors, are an important source of air pollution that is difficult to monitor and control. Within industrial facilities such as oil and gas processing plants, fugitive methane emissions can be a significant source of greenhouse gas emissions. In Brazil, as in other countries, there are specific regions with high concentration of industrial activities, and showing high population density. These sites, including megacities like São Paulo, are growing in size and economic activity. At the same time, there is a remarkable growth in concerns about the environmental issues associated with these activities. In a constantly changing world, with increasing concentrations of greenhouse gases (GHGs), among them methane (CH4) and volatile organic compounds (VOC), mitigation of atmospheric emission these gases to contain global warming, is of key concern, gas data suggest that fugitive emissions accounted for more than 5% of global greenhouse gas emissions over the past 5 years. Optical remote sensing techniques as lidar can attend the need for real time and trustable information on fugitive emissions. These techniques are non-intrusive, of relative simple construction, thus demanding less maintenance, and are able to provide data from distant locations with a high spatial resolution, typically up to 20 km from the measuring local, and 3 to 4 m long segments. Besides, information on different pollutants can be obtained simultaneously by adequate optical arrangements and data treatment methods. The technique can supply adequate information at lower costs and less effort than other techniques. The Cavity Ringdown Laser Spectroscopy (CRDS) technique was adopted because it is widely used in the detection of gas samples that absorb light at specific wavelengths and also for their ability to detect mole fractions up to the parts per trillion level. The correlation of the data between the techniques of real-time detection becomes interesting, since practical operations, fast and with a high level of sensitivity and precision are made. The mixing ratio of CH4 can be observed within the planetary boundary layer. The measured methane profiles correlate with the acquisitions made with the CRDS, however, an additional contribution of control data in which the Raman lines detect with high sensitivity.

Parallel session topic: *Transport Phenomena* **# A.2.1**

Transport properties of CH4/CO2 gas mixtures in oil and gas industry

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Keywords
Natural gas, Supercritical properties, Force fields, Molecular scale.

Impact statement
Within the realm of natural gas innovation, it is indispensable to identify the thermophysical properties for fluid mixture under the operational condition for numerous procedures and purposes. Therefore, the computer simulation methods could provide a cost-effective and reliable alternative for investigating the supercritical properties of fluids.

Highlights
'- The transport properties of pure methane, pure carbon dioxide, and their mixtures have been discussed. - Molecular scale simulation techniques are used for predicting physical properties. - Force fields for modeling methane and carbon dioxide have been chosen and validated for properties of interest. - A comparison of the computed properties with the available literature data has been done.

Abstract
During recent years, lack of reference data for describing CH4/CO2 mixture properties at supercritical states has been noticed by researchers due to its numerous applications in the natural gas exploration and processing, carbon capture and storage (CCS), among other subjects. In the present work, the transport properties of pure methane, pure carbon dioxide, and their mixtures have been discussed at pressures and temperatures that are useful in the natural gas industry. Molecular scale simulation techniques are of interest for predicting physical properties. The most important step in computing properties is to choose force fields precisely for modeling methane and carbon dioxide. For this purpose, rigid and flexible force fields are proposed in the literature. Density is the first important property to be examined and validated by employing an appropriate force field. A comparison of the computed properties with the available literature data is discussed in details to demonstrate which kinds of force fields are capable of predicting physical properties at pressure and temperature ranges under supercritical conditions.

Parallel session topic: *Transport Phenomena* **# A.2.2**

Centrifugal Impeller Design using the Topology Optimization Method

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Keywords
Topology Optimization; Centrifugal Impeller; Adjoint Method

Impact statement
In this work, the Topology Optimization Method is being used to design impeller for centrifugal flow machines. Designs being obtained are very different from traditional ones and very few information is needed to design an impeller using this methodology.

Highlights
The continuous adjoint approach is used to calculate sensitivities in a rotating coordinate frame
Cyclic boundary conditions are used to represent a sector of a centrifugal impeller
Minimization of energy dissipation inside the impeller is considered as objective function
3D examples are presented

Abstract
In Carbon Capture and Storage (CCS) processes, CO2 is captured from its main sources, transported through pipelines and stored in safe places. Usually, deep geological formations are considered for storage, so transportation and injection of CO2 require high working pressures. This can be achieved with the use of pumps and compressors and results in a Supercritical condition for the CO2 (pressure and temperature higher than critical point). A methodology to apply the Topology Optimization Method to design centrifugal impellers for Supercritical CO2 is being developed and, in this work, the latest advances are presented. Flow simulation is performed by solving the Navier Stokes equations in a rotating coordinate system. The Finite Volume Method is being used with the open source library OpenFOAM. Optimization of the impeller is conducted with the Globally Convergent Method of Moving Asymptotes (GCMMA). Sensitivities are calculated with a continuous adjoint approach. The representation of the impeller is made only by a sector, so it is assumed that the flow is repeating itself in a rotational pattern (with respect to the rotation axis). Examples of impeller designs obtained by this methodology are presented and a comparison of an optimized impeller with a traditional design is performed.

Parallel session topic: *Transport Phenomena* **# A.2.3**

Sensitivity Analysis of the blade angles and thicknesses of an Air Centrifugal Compressor Impeller

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Keywords
Elementary effects, Centrifugal compressor, Sensitivity analysis, Numerical SImulation

Impact statement
This work can contribute to find the main input variable which impact on centrifugal compressor performance. The Screening Sensitivity Analysis is a powerful tool to reduce the significant number of input variable in order to focus the numerical analysis only on important parameters reducing the processing time and increasing the knowledge of the dynamic flow.

Highlights
Screening Sensitivity Analysis is a powerful tool to reduce geometrical input variables; Thickness and angles are both important on impeller centrifugal compressor performance; The geometrical input variable impact at different level on temperature ration, pressure ratio and isentropic efficiency.

Abstract
The centrifugal compressors performance is influenced by geometric input variables such as blade angles and thicknesses. This type of geometric variable can enhance some dynamic phenomena as shock waves, boundary layer detachment and swirl. The impact of several inputs on centrifugal compressor performance could be assessed by a Sensitivity Analysis which is an important screening tool for large models, speeding up the process of machines enhancement and providing non-intuitive insights of the physical model. Thus, in order to determine the influence of the blade thicknesses and angles on the overall performance of an impeller, an Elementary Effects (EE) screening sensitivity analysis associated to a robust CFD model using ANSYS CFX was performed based on NASA CC3 turbocompressor impeller 4:1 (using air as working fluid). The feasible region for an impeller CFD model can be strict depending on which type of input variable has being modified, which can result in different sample space ranges for thicknesses and angles. For the present analysis, the thickness and angle range is 20% and 1%, respectively, related to its nominal values. Those different ranges have an important role in EE sensitivity indices calculation, since this global sensitivity analysis method takes into account the whole sample space variation. Results have shown that the two blade thicknesses and two blade angles, at a medium spanwise position, were responsible for about 72% and 28% of isentropic efficiency variations, respectively. However, this scenario changes for input power and temperature ratio where the angles are responsible for about 75% of variations. Pressure ratio demonstrated to be influenced similarly for both types of variables. Although the blade angles have an input space range 20 times smaller than blade thicknesses it is considered a very important variable for the impeller design. Furthermore, the screening sensitivity analysis should always consider a broader range for all input variables, which could contribute to define a robust surrogate model training in order to feed support an optimization procedure.

Parallel session topic: *Transport Phenomena* **# A.2.4**

Thermodynamic analysis of multi-stage compression system for CO2 injection

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Keywords
supercritical CO2; multi-stage compressor; thermodynamic model; CO2 injection;

Impact statement
Applying optimization process to find the optimum operating conditions of a CO2 injection unit leads to reduced energy consumption and lower CO2 emission.

Highlights
Real data of CO2 injection unit operating in the Brazilian pre-salt basin has been used; The power consumption of CO2 injection unit is reduced by up to 3.9% with proper selection of stage pressure ratios; Pressure drop produced by intercoolers are considered in calculations; Three and four stages are simulated and compared using pure CO2, pure CH4 and a mixture of 70% CO2 and 30% CH4;

Abstract
The injection of CO2 in oil reservoirs is used by the oil and gas industry for the reduction of environmental impact and enhancement oil recovery (EOR). The compression systems used for this task work with CO2 in supercritical condition and are energy-intensive equipment. The multi-stage intercooling compression is the most traditional approach for this application, that demand high total pressure ratios. The use of optimization to find the optimum operating conditions leads to reduced energy consumption and lower CO2 emission. This work presents a comparison of two different thermodynamic models to estimate the power necessary in each compressor stage in a multi-stage compression system used in petroleum industry. The first model was implemented in C# computer language and uses an open source library for determination of thermodynamic properties: Coolprop. The second model uses Aspen HYSYS® with GERG 2008 equations of state (EoS), which were developed by the Groupe Européen de Recherches Gazières (GERG). The number of stages and pressure ratio in each stage are parameters that influence the total power required by the compression system. The use of three and four stages are investigated in this paper. The pressure drop between stages is an input parameter used to obtain inlet pressure at each stage. An optimization procedure is performed to achieve the optimum operating pressure ratios of a CO2 injection unit in order to minimize the total power consumption. Three different compositions with the variation of CO2 content: pure CO2, pure CH4, and 70% CO2 + 30% CH4. This last composition is typical in offshore platforms that separate CO2 for reinjection. In the first thermodynamic model, a MATLAB function is used for the optimization. The second model used the Genetic Algorithm of Esteco modeFRONTIER to minimize the total power consumption. The optimum pressure ratio presented a reduction in power consumption up to 3.9% when compared to a conventional operating condition.

Parallel session topic: *Market and Modeling* **# A.3.1**

A Multiperiod Peak Period Model for Electricity Planning in Brazil Under CO2 Emission Constraints

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Keywords
CO2 emissions; electricity matrix; multiperiod optimization

Impact statement
This study addresses the long-term planning for the electric power mix in Brazil considering the supply and demand during the peak periods. It is verified that the increase in the supply expansion of some renewable the non-renewable sources is a critical issue in order to meet the increasing electricity demand and CO2 emissions constraints along the next 15 years.

Highlights
A multiperiod optimization model is developed to plan the Brazilian electricity matrix. The model considers the peak periods and the dry and wet seasons. The goal is to minimize the total cost, satisfying the power demand and CO2 emission constraints. We apply the model for the electricity planning in Brazil for the years 2019-2033.

Abstract
A major challenge in electricity markets is to achieve an electricity mix that presents a high level of energy security within a range of affordable costs and environmental constraints. The use of multi-period optimization models for energy planning under environmental constraints have been receiving lately a great deal of attention. Most of the papers deal with the an annual average production and demand of electricity. However a key issue in electricity planning is to consider the supply and demand during peak periods. This study seeks to find optimal portfolios of electricity supply considering the supply and demand conditions for the peak period of the electricity system in Brazil. That is, instead of calculating the portfolio of average consumption or instantaneous power, the portfolio seeks to meet the average consumption during the period of greatest consumption, taking into account the different seasons. This is a critical issue when the electricity matrix is highly dependent on renewable sources (hydroelectricity, wind, biomass, PV) like in Brazil, so that the energy matrix has a significant change in the dry and wet periods. The model seeks to minimize the total cost (the sum of the fixed and the variable running costs) while satisfying all the electricity demand, maximum supply and maximum greenhouse emission in the dry and wet seasons. This study considers different scenarios, one with expansions constraints as expected for the next 15 years, and the others with more flexible expansion possibilities. It was verified that the increase in the supply expansion of some renewable the non-renewable sources is a critical issue in order to meet the increasing electricity demand and CO2 emissions constraints along the next 15 years.

Parallel session topic: *Market and Modeling* **# A.3.2**

Analysis of the potential Liquefied Natural Gas market for Brazil: The case study of Mato Grosso state

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Keywords
Liquefied Natural Gas; Market; Mato Grosso

Impact statement
A new consumption market for natural gas is relevant to keep the Bolivia/Brazil energy integration and the results showed us that there is a potential natural gas market in Mato Grosso State. However, the access to the points of consumption requires less conventional logistics solutions, such as small-scale Liquefied Natural Gas production and its transportation by road.

Highlights
Mato Grosso state (MT) economic relevance: MT energy source: fuel oil, diesel and electricity, Presence of an international natural gas (NG) pipeline from Bolivia to MT capital state, but lack of NG distribution pipeline to MT countryside area Results:the potential NG consumption volume and the Capex and Opex to transport the Bolivian gas to the countryside area transported trought LNG by road

Abstract
The aim of this work is to analyse the Bolivian natural gas additional market in Mato Grosso state through of the economic sector as a potential consumption volume, and operational expenditure costs to transport the Bolivian gas to the Mato Grosso state, replacing diesel, electricity, and fuel oil with liquefied natural gas transported by road and serving the agricultural, industrial and transportation sectors. Base on in this context, although Natural Gas has a minimal share in Mato Grosso energy source matrix, in the late 1990s a group of investors developed the Cuiabá Integrated Project (PIC), including the construction of a thermal power plant at the capital of the state called Cuiabá, and the construction of a natural gas pipeline from Bolivia country to Cuiabá city in the context of the energy integration between both countries. However, due to recent legal issues involving the Cuiabá thermal power plant' owner, the Bolivia Mato Grosso gas pipeline is out of operation. In additional, the natural gas supply agreement between Brazil and Bolivia is about to be closed and there are some doubts if the Brazilian government wish to renew the same currently natural gas volume. The case study uses the methods described by Gallo (2018) and Strapasson (2004) to estimate the potential Liquefied Natural Gas demand in the Mato Grosso state and uses the Cost Estimate Model for calculating the Liquefied Natural Gas transportation costs by road proposed by Fraga (2018). The total cost per energy unit (MMBtu) of the entire Liquefied Natural Gas transportation chain is estimated, which is supposed to be liquefied in a small-scale liquefaction unit and transported in Liquefied Natural Gas trucks up to five points of consumption in the state of Mato Grosso.

Parallel session topic: *Market and Modeling* **# A.3.3**

Biogas and biomethane potential for municipalities in Sao Paulo State

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Keywords
Biogas, biomethane, electric power

Impact statement
Despite the huge potential for biogas and biomethane, current situation of existing projects shows a extremelly short number. The huge potential assessed for the state municipalites is important to attract potential investors and to allow the development of adequate policies. Considering that this production is from residues, there is an important synergy with basic sanitation.

Highlights
The highest potential is in the sugarcane sector, to be produced from sugarcane processing residues. The biomethane potential for the state allows a surplus of 3.87 billion Nm3, after supplying all NG consumption in the state In another option, it could replace 72,4% of the diesel consumption The electric power that could be produced is equivalent to 93% of residential consumption in the state.

Abstract
The objective of this project is to analyze prospects, the corresponding benefits and potential barriers and to propose appropriate policies for integrated solutions using biogas and biomethane in the energy matrix of Sao Paulo State. After a detailed revision and update of the processes involved in biogas and biomethane production and use, the project assessed the biogas, biomethane and electric power potential for each municipality in the state, considering the main sources available: urban and rural residues, as well as the available by-products from sugarcane process (vinasse, filter cake and tops/leaves). Urban residues included the organic fraction of municipal solid waste (MSW) in landfills and sewage from liquid treatment stations. Rural residues included main animal residues (bovines, swines and poultry). The potencials were evaluated for each source and for each municipality, presented in a geo-referenced map, including all alyers related to infrastructure (electric grid, sub-stations, natural gas grid, compressing stations) and conservation units in the state. Results show significant figures for potential mainly considering the few biogas/biomethane plants in the state. Only five landfills produce electricity from biogas with an installed power of 80 MW, against a potential equal to 418 MW. In the sugarcane sector, after several previous experiences not successfull, there are now only three projects for biogas production (Iracema mill), for biogas-based electricity (in Bonfim mill), for biomethane production and use (Cocal mill and Gas Brasiliano). On the other hand, the potentials for biogas, biomethane and electric power for the sector is huge. The potential fo biomethane production in the sector reaches 7.85 billion Nm3/year, allowing a surplus of 2.82 billion Nm3, after supplying all NG consumption in the state. Authors are grateful for the support of RCGI - Research Center for Gas Innovation, located at the University of São Paulo (USP) and funded by FAPESP - São Paulo State Research Support Foundation (2014 / 50279-4) and Shell Brasil, and the importance of the support given by the ANP (National Agency of Petroleum, Natural Gas and Biofuels) through the regulatory incentive of R & D. We would also like to thank ABIOGAS, DATAGRO, EPE, CiBiogás, SABESP and Gasbrasiliano for providing some of the information necessary to perform the calculations and the preparation of the maps.

Parallel session topic: *Market and Modeling* **# A.3.4**

NATURAL GAS MARKETING AND COMPARATIVE ANALYSIS WITH THE FREE ELECTRICITY MARKET

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Keywords
Commercialization; Electricity; Natural Gas

Impact statement
There is a need for the establishment of a new design of the natural gas market, especially in relation to the determination of rules for unregulated commercialization, coupled with the continuous growth of the free market for the commercialization of electric energy, it is justified to analysis of the main aspects related to the commercialization of natural gas in the secondary market.

Highlights
Can the distinct historical and institutional aspects, as well as the constitutional provision of state exclusive competence for the distribution of piped gas, represent obstacles to the commercialization of piped gas within the molds of the electric sector?

Abstract
The energy sector is a driver of a country's economy and social development (BOECK, 2014). Thus, with the current forecast of the consolidation of the growth of the Brazilian economy and the increase of confidence in the current policy, it is indispensable for the public power to adopt measures that allow the increase capacity of supply and demand of production, in order to mitigate any existing bottlenecks, as the possible inefficient energy supply. According to studies initiated under the Gas to Grow initiative (MINISTRY OF MINES AND ENERGY, 2016), regulatory adjustments target the diversity of players in the sector, competitiveness, attracting investments, liquidity, access to information, the greatest dynamism. , good national and international market practices, compliance with contracts and, especially, the viability of the free natural gas market. Many of these discussions involving the commercialization of natural gas in a free market result in the regulatory structuring of this environment, possibly using regulatory parameters related to the contracting already adopted for the structuring of the free electricity market. In this context, in which there is a need for the establishment of a new design of the natural gas market, especially in relation to the determination of rules for unregulated commercialization, in conjunction with the continuous growth of the free market for the commercialization of electricity, it is important to emerge. Question: What conditions in the free market for electricity can be taken advantage of in the free market for natural gas? The objective of this research is to compare, especially from a regulatory point of view, the markets for the free commercialization of electricity and natural gas and to analyze, from the available information, the feasibility of adopting the regulatory model of the electricity sector to the natural gas sector. that partially. The methodology to be employed in this research is the analysis of the comparative between the free energy and natural gas markets, from the regulatory and legal point of view. To this end, the relevant literature, normative acts, such as laws, decrees, resolutions and ordinances are analyzed, as well as reports and technical studies carried out by sectoral institutions, such as MME, ANEEL and ANP.

Parallel session topic: *Transportation* **# B.1.1**

Natural gas use in the transport sector of São Paulo State: environmental benefits in 2035

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Keywords
Natural Gas, Freight transport; LEAP model

Impact statement
This paper contributes to the current debate on the need for new options for freight transport. In Brazil, the only fuel available for freight in heavy-duty trucks is diesel. With this, there is great dependence on a single fuel, which creates a monopoly around diesel use. This study brings an important discussion around the use of natural gas and its environmental benefits if used in heavy-duty.

Highlights
This study focuses on freight Natural gas provides reductions in Nox and PM, but depends on the modal There is no consensus on the actual benefits of natural gas

Abstract
São Paulo state is an example of the importance of tackling regional energy systems. While GHG emissions from the energy sector in Brazil corresponds to 21% of total emissions, in São Paulo the share is 51% and, in the land use sector, emissions reach 46% in the country and only 9% in the state of São Paulo. Within the energy system, special attention must be given to the transport sector, which corresponds to 54% of emissions from the energy sector. Using LEAP model, this study aims at estimating greenhouse gases and pollutant emissions from freight transport by 2035 with a 10% substitution of heavy and light duty vehicles in the state of São Paulo. Results show that greenhouse gases reductions are almost neglectable in a 10% substitution, mainly due to increase in methane and nitrous oxide emissions. Pollutant reductions are seen in particulate matter in both heavy and light duty vehicles. Nitrogen oxides and carbon monoxide, on the other hand, increase in light duty and decrease in heavy duty. Hydrocarbons increase in both modals.

Parallel session topic: *Transportation* **# B.1.2**

LNG as Fuel for Inland Navigation: a case study for the north region of Brazil

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Keywords
lng as fuel; inland navigation; energy efficiency

Impact statement
A study regarding the application and benefits of replacing conventional fuels by LNG in the north region of Brazil is presented, focused on the inland navigation. A simulation tool was developed applying state-of-the-art mathematical modeling of the complete navigation. The tools was validated considering fuel scale data collected from real vessels.

Highlights
A navigation simulation tool was developed focused on inland navigation in the North region of Brazil. The benefits of replacing the conventional fuel by LNG is estimated according to the "real" operational profile of the vessel. The numerical model is validated using real data collected from the vessel, as environmental conditions measured in loco.

Abstract
In this study three main aspects were investigated: The implementation of a performance simulator for hybrid vessels, the development of a technical criteria to select and dimension a battery set for hybrid vessels and the concept design of a LNG fueled inland push-barge convoy. The push-barge inland convoy study has started in the first quarter of 2018 with the suggestion of the Houston based Shell group and, during this period, the involvement of Cargill, an international grain market operator and of the Sotreq group (Caterpillar) were brought into the project. The initial discussions with the partners involved the understanding of the basic characteristics and requirements of the logistic and operational procedures applied to the Brazilian North Inland Waterway (IWW) along the oriental part of Amazon River. A performance simulator was developed considering the environmental conditions and vessel operational data. The real vessel is modelled considering the installed equipments to convert the power demanded by each propeller into the demanded electric loda (electric motor, VFD, transformer, switchboard, generator, internal combustion engine are modelled). The ship resistance is estimated based on literature regressions and CFD models considering the shallow water effects. The river flow is also discretized in space and time to allow a sensitivity analysis regarding the seasons of the year. The simulator was validated with collected data in order to provide reliability to the numerical predictions. The tool is then applied both to estimate the possible benefits of applying LNG as fuel instead of the conventional fuels applied as the benefits of a battery pack in the operational profile of the vessel.

Parallel session topic: *Transportation* **# B.1.3**

Development of a Hybrid Vessel Simulator

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Keywords
hybrid; propulsion; simulation

Impact statement
Propulsion of diesel-powered vessels has found difficult to adjust economically to rising fuel costs, environmental legislation to reduce air pollution and the introduction of carbon dioxide taxes. Thus, a PSV (Platform Support Vessel) hybrid vessel system is developed to reduce emissions and increase engine efficiency to adapt the system performance within emission-constrained port regions.

Highlights
Integration of electric and energetic models of hybrid power systems to the maritime mission simulator developed and maintained by the research group of the Numeric Offshore Tank (TPN) at the University of São Paulo. Tool intended to validate the developed models and test optimized solutions. The model takes the dynamics of the power system into consideration in the simulation.

Abstract
The propulsion for merchants ships nowadays, it is dominated by diesel machines, where the principal costs for the ship operation is the fuel. Naval industry workers are questioning the sustainability of the current propulsion due the factors: the increasing fuel costs, the environment legislations for reduce the air pollution and the introduction of taxes for the carbon dioxide emission. Alternatives fuels with low Sulphur content, as the Liquefied natural gas (LNG), are an option to be considered to reach the pollutant reduction. The LNG can be utilized in combustion engines, as the convectional piston motor or a reaction motor. This present project has as objective the integration the electric and energetic models developed inside the RCGI Project 7 (Power hybrid systems for ships) to the maritime mission simulator developed by the research group of the Numeric Offshore Tank (TPN) with aim to validate the developed models and test optimized solutions. The model are composed by four principal parts: the internal combustion engine (which can utilize natural gas and/or diesel as fuels), generator and fuel cells; the electrical part, encompassing the batteries, the transformer, the electric motor and its velocity controller; the propeller dynamic part, which is composed by the propeller generated forces model; and the dynamics of the ship, calculating its current velocity and the hybrid supervisory control part. The system has the capability to propel the ship utilizing the batteries stored energy during a time that depends on the required velocity. The hybrid supervisory control observes the solicitation and the amount of charge in the batteries, being able to turn on the generator moved by LNG. The system was modelled and tested using the software Matlab and presented satisfactory results since each component worked as desired. The algorithm has good execution performance, reaching the average execution time of 0.01 seconds for each time step, well under the execution-sampling period of the simulator that is of 0.1 seconds. We make a study considering two scenarios. The first is a fast 30 minutes pre scripted trip in high sea, where is modified the number of batteries and its efficiency, being compared to a two non-hybrid vessel, one using only a Diesel motor and other using an LNG/Diesel motor. The second scenario it is a 15-hour long trip in high sea, to test the robustness of the model for long pre script trips.

Parallel session topic: *Transportation* **# B.1.4**

Use of Variable Speed Diesel Generators to reduce CO2 emissions in Platform Supply Vessels

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Keywords
Variable-Speed Generators; Ship Power Systems; CO2 Emissions

Impact statement
According to the latest report of the European Commission, ships were responsible for around 2% of the global CO2 emissions; it places the shipping sector as the 7th biggest emitter of CO2. Our work pursues some analysis aiming at verifying the impact of the variable speed diesel generators on the ship power system.

Highlights
We analyze the impact on CO2 emissions of various configurations involving 1.8MW diesel engines and 450kW diesel engines being operated at variable and fixed speed with and without batteries. The impact of these configurations in each part of a standard routine of the PSV is also measured.

Abstract
Greenhouse gases emissions are one of the most critical worldwide concerns, and multiple efforts are being proposed to reduce these emissions. Shipping represents around 2 % of the global CO2 emissions. Since ship power systems have a high dependence on fossil fuels, hybrid systems using diesel generators operating variable speed are becoming an interesting solution to reduce emissions. In this work, we analyze the potential implementation of Li-ion batteries and auxiliary diesel engines in a platform supply vessel system through simulations using HOMER software (Hybrid Optimization Model for Multiple Energy Resources).

Parallel session topic: *Fuel cells* **# B.2.1**

Unveiling Fundamental Transport Phenomena in Fuel Cells

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Keywords
Fuel Cell; Catalyst Layer Utilization; Oxygen Imaging

Impact statement
The results highlight the need to carefully consider non-convenctional variables when developing fuel cells, and that a compromise between performance and durability might be needed. The coupling of thoroughly established techniques with a new and versatile tool displayed in this work, can pave the way to minimize such trade backs in the quest for efficient and durable practical PEFC devices.

Highlights
In situ and ex situ spatially-resolved techniques; Reactant distribution impacts in a polymer electrolyte fuel cell; Contribution of convection in heat as well as reactant distribution; Water build-up from neutron tomography is linked to component degradation; Local current densities might shape degradation patterns in fuel cells;

Abstract
In situ and ex situ spatially-resolved techniques are employed to investigate reactant distribution and its impacts in a polymer electrolyte fuel cell. Temperature distribution data provides further evidence for secondary flows inferred from reactant imaging data, highlighting the contribution of convection in heat as well as reactant distribution. Water build-up from neutron tomography is linked to component degradation, matching the pattern seen in the reactant distribution and thus suggesting that high, non-uniform local current densities shape degradation patterns in fuel cells. The correlations shown between different techniques confirm the use of the versatile reactant imaging technique, which is used to compare commonly used flow field designs. Among serpentine-type designs, the single serpentine is superior in both equivalent current density and reactant distribution, showing large contributions from convective flow. On the other hand, the interdigitated design is shown to produce larger equivalent current densities, while showing a somewhat poorer reactant distribution. Considering the correlations drawn between the techniques, this suggests that the interdigitated design compromises durability in favour of power output. The results highlight how established techniques provide a robust background for the use of a new and flexible imaging technique toward designing advanced flow fields for practical fuel cell applications.

Parallel session topic: *Fuel cells* **# B.2.2**

A hybrid serpentine-interdigitated flow channel geometry for fuel cells

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Keywords
fuel cell; flow channel; simulation

Impact statement
While a proposal, the new flow channel geometry may bring long seeked improvements to fuel cell devices by tuning only one cell component. In addition, it may further corroborate a mixed computational-experimental approach based on device analogues, allowing fuel cells to be studied and improved at a much lower cost.

Highlights
Reaction utilization comparable to interdigitated. Pressure drop comparable to serpentine. Flow field may suggest good water removal. Potential for optimization. Device independent.

Abstract
Fuel cells have impressive potential for decarbonization and as high efficiency power sources, however many challenges have yet to be addressed for large scale deployment and uptake. Among the many noteworthy lines of research underway, investigating the best flow field in a given device has been carried a number of times, with perhaps limited success regarding performance improvement. As a possible final attempt to look over such matters individually, from the component point of view, we propose yet another flow channel geometry for small-scale fuel cells, in particular polymer electrolyte fuel cells (PEFCs). The proposed geometry incorporates elements from the two most studied geometries, namely single serpentine and interdigitated. The rationale is that serpentine channels have large pressure drop, thus aiding in water removal, while interdigitated promises to deliver large quantities of reactants to the catalyst. However both seem to fail where the other excels, and thus devices are left to compromises. The new geometry, as well as its inspirations, are simulated in a previously validated computational model, further improved and with high spatial resolution, of a prototype PEFC cathode. The model is isothermic, non-electrochemical and disregards water, as the experimental system. However it has been shown to be useful when studying PEFCs, and a secondary goal of this work is to corroborate this. Comparing simulation results between geometries, it is seen that the hybrid geometry does inherit the characteristics of interest, i.e. high reactant utilization and pressure drop, suggesting it may be of use in real PEFCs. Finally, a niche application is proposed based on the reaction rate distribution of the hybrid geometry.

Parallel session topic: *Fuel cells* **# B.2.3**

Reducing the sintering temperature of solid oxide fuel cells by controlling the shape of ceria-based eletrolyte nanoparticles

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Keywords
solid oxide fuel cells;
nanoparticles, shape control

Impact statement
The broad impact is the reduction of cost and enhanced performance of intermediate temperature solid oxide fuel cells. Specific impacts are related to the development of cost competitive synthesis methods that allow for the sintering of dense ceria-based electrolytes (> 93% of theoretical density)at temperatures below 1200 C.

Highlights
A simple chemical method was developed for producing ceria-based nanoparticles with high sintering activity. Sintering of dense gadolinia-doped ceria electrolytes at 1150C Fuel cell tested underH2 showed promising performance

Abstract
The development of solid oxide fuel cells operating at intermediate temperature (IT-SOFCs) and using carbonaceous fuels to generate power have been crucial for the widespread commercialization of SOFCs. Gadolinium-doped cerium oxide (CGO) is known to display the desired properties to be used both as a high ionic conductor electrolyte at intermediate temperatures and as an active layer in the anode due to its catalytic properties for the decomposition of fuels containing hydrocarbons. In this study IT-SOFCs were fabricated with highly reactive nanorods of CGO electrolyte powder with shape controlled by a hydrothermal synthesis developed in this project. The tested fuel cell system consists of the CGO electrolyte support, lanthanum strontium cobalt ferrite (LSCF) cathode and Ni/CGO anode. The performance of the cell was evaluated with hydrogen as a fuel and air as an oxidant at temperatures between 500–700 °C, further work will be carried out to evaluated the performance of the cell when operating with natural gas. The experimental results indicate that a high-performance IT-SOFC can be obtained with a relatively low temperature (1.150 C) two-step sintering of the ceria-based layers.

Parallel session topic: *Fuel cells* **# B.2.4**

Gas properties within Carbon Nanotubes

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Keywords
membranes, carbon nanotubes, molecular dynamics simulations

Impact statement
The emergence of the nanostructured carbon-based materials could lead to optimal phase separation devices due to their fast mass flow and regular pore size. Based on molecular dynamics simulations, we investigated the underlying molecular mechanisms which may lead to the phase separation and influencing nanoflows of natural gas within carbon nanotubes.

Highlights
Molecular dynamics simulations applied to the gas industry problems. Design smaller and more efficient materials for separation purposes. Gas selectivity, diffusion, exchange rate, charge density profile, gas distribution, orientation and the relationship of these features with nanotube diameter and gas composition.

Abstract
Improvements in natural gas separation technologies are highly desirable, considering current membrane systems that display low flow rate accompanied by low selectivity and vice versa. Such devices often occupy a huge area in an industrial plant, which is an undesirable feature in offshore platforms. Therefore, one of the challenges encountered in the Oil & Gas industry is to design smaller and more efficient materials for separation purposes. Advances in nanotechnology brought a new perspective to this challenging problem. In particular, carbon-based materials, i.e carbon nanotubes and graphene, can lead to optimal devices due to their extraordinary features, such as their regular pore size and fast mass transport. Such systems may involve nanoconfinement geometries and interfacial effects controlling fluid properties. In this context, computational approaches at the atomistic level could provide essential knowledge about confinement interface features. By using fully atomistic molecular dynamics simulations, we investigated the structure and transport of carbon dioxide, methane and their mixture within the carbon nanotubes. We explored gas selectivity, diffusion, exchange rate, charge density profile, gas distribution, orientation and the relationship of these features with nanotube diameter and gas composition. We evaluated confinement effects by comparing the spatially constrained fluids against the bulk phase properties. It was found that gas species are distributed heterogeneously inside the tube. This feature is attributed to interface effects and the adsorption affinity differences displayed by the molecules at the carbon nanotube's surface. The gas selectivity variations observed at the surface layer and middle pore revealed that spatial confinement could lead to the natural gas phase separation within the carbon nanotubes. In summary, we could evaluate the underlying molecular mechanisms which could lead to gas filtering. These results may lead to the development of suitable membranes that can optimize gas separation processes.

Parallel session topic: *Policies and Regulation 1* **# B.3.1**

The strategies of Bioenergy Carbon Capture and Storage (BECCS) and the role of Brazil and its New Biofuel Policy, RenovaBio

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Keywords
BECCS, RenovaBio, sugar cane

Impact statement
According to available literature and the Intergovernmental Panel on Climate Change (IPCC), capturing the carbon generated by biomass and stocking it may result in negative emissions. Also, capturing CO2 from renewable sources can be cheaper than from fossil sources because some renewable energy process of conversion deliver practically only CO2, reducing costs with treatment of emissions gases.

Highlights
The production of second generation ethanol and synthetic natural gas (bio-SNG), anaerobic digestion and production of industrial compounds such as methanol and synthetic fuels are listed as key processes for BECCS. RenovaBio can favor Brazil as a supplier of environmentally friendly biomass or encourage the production of less emitters biofuels, including the application of BECCS.

Abstract
The Bioenergy with Carbon Capture and Storage – (CCS) and Bioenergy with Carbon Capture Utilization and Storage (CCUS) emerge as a mechanism to mitigate climate change because they offer cheaper and more efficient alternatives to capture GHGs compared to CCS applied to fossil fuels. This article focuses on the concept of negative emissions, as well as issues such as availability of Brazilian biomass for this new market, especially from the sugar and ethanol industry, taking into account the weight it has on energy and electrical Brazilian matrices, since this biomass is already used for cogeneration and power generation. The article still contextualizes this technology within the new National Biofuels Policy.

Parallel session topic: *Policies and Regulation 2* **# B.3.2**

Brazil's New Role in the Global Climate and Energy Governance

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Keywords
Brazil, Energy, Climate Change, Governance

Impact statement
Until recently, Brazil has standed out in global climate and energy governance due to some successful initiatives to preserve the environment and due to its "clean" energy mix, with a large share of renewable sources. These factors, however, are changing. Our goal is to understand how the country will deal with that in the international arena and what are the impacts domestically

Highlights
Brazil's shifting position in the global climate and energy governance.
Is Brazil a new major energy player?
The future of Brazil's GHG emissions and the impacts on climate change negotiations.

Abstract
Brazil has been a leading actor in global climate governance. Since the beginning of the 1990s, the country has hosted some of the most important conferences on environment and development, and taken the lead in proposing initiatives such as the Clean Development Mechanism (CDM), the Amazon Fund, and the principle of Common but Differentiated Responsibilities (CBDR). After Jair Bolsonaro's election, however, the country's traditional position on the issue has been going through fast and considerable changes. On the energy side, as well, Brazil's role has also been changing. The new-found petroleum reserves, discovered in the pre-salt layer, may soon convert the country in a major world oil and gas exporter, raising expectations that it will soon adapt its position in the global climate and energy governance according to its new resources and capabilities. Our goal is to analyze the opportunities and risks for Brazil before these new scenarios.

Parallel session topic: *Policies and Regulation 3* **# B.3.3**

Carbon Capture and Storage (CCS) in Brazil: a comprehensive analysis of the challenges for implementation through a Socio-Technical Framework.

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Keywords
Carbon Capture and Storage (CCS); Socio-Technical; Energy Transition

Impact statement
This paper presents a framework to be considered in CCS implementation projects, which is comprehensive in the main challenges to be analysed, related to the uncertainties in the technical, environmental, economic, legal and social dimensions.

Highlights
Energy transition requires a comprehension of the challenges involved in CCS implementation.
The challenges of implementing CCS in Brazil reach a broad range of perspectives.
A social-technical approach allows considering technical, environmental, economic and social dimensions.
Multidisciplinary and integrative views are the best path to tackle complex problems.

Abstract
Carbon Capture and Storage is a relatively new technology that is being implemented in some parts of the world in order to contribute towards the mitigation of greenhouse gases and their effects on climate change. This work is focused on discussing the main challenges involved with the implementation of such technologies using a socio-technical approach. Through a comprehensive framework, this paper considers seven uncertainties related to CCS application to analyse the Brazilian environment. These uncertainties cover aspects in the areas of pathways variety; storage safety; deployment and development speed; the CCS systems integration; the viability considering economic and financing aspects; regulatory and policy perspectives; the public perception in general and in specific audiences. This socio-technical methodology explores the gaps to be taken into consideration when analysing Brazil CCS development. It reinforces the need to approach the challenges in a broad perspective, regarding technical, environmental, economic and social aspects. Energy transition to a low carbon economy is discussed based on historic evolution to understand the present challenges. The Research Centre for Gas Innovation is the illustrative case by which it is possible to demonstrate the relevance of an integrative approach involving technical solutions together with environmental, social and economic visions, more specifically discussed by the analysis of the CO2 abatement projects.

Parallel session topic: *Policies and Regulation 4* **# B.3.4**

Compliance of CCS Activities in Climate Change Policies in Brazil

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Keywords
Climate Change; Carbon Capture and Storage; GHG Emission mitigation

Impact statement
There is still no forecast for how the government will incorporate the recommendations in the development of the NDC Implementation and financing Strategy (SEEG, 2018). There is the possibility that issues related to CCS activities, implementation, regulation, monitoring and permission, for example, may be framed in the tasks of the CIM and its role in National climate Change plan.

Highlights
Ordinance No. 150 of 2016, establishing the national plan for adaptation to climate change
Brazil has an Interministerial committee on Climate Change (CIM) with the role of guiding the elaboration, implementation, monitoring and evaluation of the National Plan on climate change
In the context of the CIM, the Executive Group on Climate Change was established in order to elaborate, implement.

Abstract
The present article aims, based on the deductive methodology, and normative and bibliographic analysis, to demonstrate elements that corroborate the thesis that the governance of CCS activities in Brazil are supported by the existing configuration proposed for the Policies aimed at climate change in the country.

Parallel session topic: *Catalysts* **# C.1.1**

CO-PROX reaction on 1-3 wt.% CuO/CeO2 catalysts: an in situ XANES study

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Keywords
CuO/CeO2, CO-PROX, metal-support interaction

Impact statement
CuO/CeO2 catalysts with 1 to 3 wt.% of copper were investigated by in situ XANES under CO-PROX reaction conditions. XANES results were compared with those of the catalytic performance of the materials. Our studies indicated that the CO-PROX reaction on CuO/CeO2 is impacted by the oxidation state of Cu species, which in turn may vary with reaction temperature, depending on the Cu content.

Highlights
Cu content of CuO/CeO2 catalysts can impact on the CO-PROX reaction. The oxidation state of Cu species in the CuO/CeO2 catalysts depends on the temperature and Cu content. Cu+1 and Cu0 seems to be active species in the CO-PROX reaction. Decreasing reaction temperature causes the oxidation of Cu species. The oxidation of Cu species may be associated with a drastic decrease of the CO conversion.

Abstract
The impact of the Cu content of CuO/CeO2 catalysts on their characteristics and catalytic performances towards the CO-PROX reaction was evaluated. CuO/CeO2 catalysts with nominal contents of 1, 2 and 3 wt.% of copper were synthesized by the co-precipitation method (CPA) and namely 1CPA, 2CPA and 3CPA, respectively. The investigated catalysts were characterized by SEM-EDS, XRD, BET, H2-TPR and in situ XANES and applied to the CO-PROX reaction. The results showed that increasing amount of Cu in the materials results in smaller crystallite size of CeO2 and higher surface area. The material reduction profiles presented two overlapping peaks below 250 °C, attributed to the reduction of surface CeO2 and CuO species. The 2CPA and 3CPA catalysts exhibited similar H2 consumption and reduction profiles. However, the 1CPA sample showed lower H2 consumption than 2CPA and 3 CPA, while the corresponding reduction peaks were shifted to higher temperatures. This difference may be due to: (1) the presence of relatively larger CuO particles and/or (2) the low copper content of the 1 CPA material, which may have caused a weaker metal-support interaction. By comparing the turnover frequency, the 1CPA sample presented worse catalytic performance than that of the 2CPA and 3CPA samples up to 145 °C, but above this temperature up to 250 °C the 1% Cu catalyst was superior to the other materials. The catalytic behavior of the samples may be related to their reduction properties, in accord with TPR results. In situ XANES analyzes under CO-PROX reaction conditions shed light to the nature of active copper species involved in the CO-PROX reaction between 120 °C and 200 °C. The investigated catalysts present a balance between Cu0 and Cu1+ species under reaction conditions, confirming the redox behavior of these materials. From these results, we can infer that active copper species include Cu0 and Cu1+ for the catalysts synthesized by co-precipitation. Furthermore, it was observed that for the 1CPA catalyst the decrease of the reaction temperature from 200 ºC to 120 ºC caused oxidation of the Cu species, resulting in a drastic decrease of CO conversion. These results show that the CO- PROX reaction on CPA catalysts is impacted by the oxidation state of the Cu species, which in turn may vary with the reaction temperature, depending on the copper content in the material.

Parallel session topic: *Catalysts* **# C.1.2**

Evaluation of catalysts supported on carbon nanotubes for Water-Gas Shift reaction for hydrogen production

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Keywords
hydrogen production; water-gas shift reaction; carbon nanotubes

Impact statement
Evaluation of new catalysts supported on functionalized multi-walled carbon nanotubes to improve the hydrogen production process via Water-Gas Shift reaction

Highlights
Synthesis and characterization of Co and Cu catalysts supported on MWCNTs were discussed
Changes in CO conversion were investigated by performing catalytic evaluation tests
The Co catalyst presented better performance, reaching near equilibrium conversions at higher temperatures

Abstract
The Water-Gas Shift (WGS) reaction is one of the most important routes for hydrogen production and for controlling H2/CO ratios in methane reforming reactions. It has received great importance due to the use of H2 in the main chemical industries (fertilizers, oil refining, etc.), fuel cells, and CO2 chemical conversion processes. Although there are already well-established industrial catalysts for the WGS reaction, such as Fe2O3-Cr2O3 and Cu-ZnO-Al2O3, for high and low temperature stages, respectively, several new ones have been developed for improving process performance and stability. For example, for portable fuel cell applications, catalysts based on noble metals at nanoscale and supported on oxides have been used due to their more resistant and suitable characteristics. In this context, the use of multi-walled carbon nanotubes (MWCNTs) as catalysts support has shown to be advantageous due to their high surface area, excellent conductivity, and the low availability of some oxides for this purpose. In the present work, the powerful features of functionalized MWCNTs were combined in two different catalysts for the WGS reaction with cobalt (Co) and copper (Cu) nanoparticles as active phases, and both promoted by ceria (CeO2) and strontium (Sr). The characterization results (N2 physisorption, XRD, TEM, Raman, TGA and TPR) were carried out to clarify the favoritism of particles deposition mainly on the support external surface, as also reported in previous works. Catalytic evaluation results showed better performance for the Co catalyst, achieving near equilibrium conversions at higher temperatures (~450oC). Therefore, these results have contributed for the work progress in order to find innovative solutions for the process improvement.

Parallel session topic: *Catalysts* **# C.1.3**

A surface science investigation of methanol synthesis on Cu-ZrO2 based catalysts

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Keywords
CO2 hydrogenation, methanol and Copper

Impact statement
CO2 has drawn widespread attention because of its possibility of CO2 recycling to produce methanol. The methanol production from CO2 abatement has been a high interest in the industry since methanol is a vital raw material for the chemical industries. In this way, several technologies have been proposed to mitigate, as it is one of the major "greenhouse gases" released into the atmosphere.

Highlights
Cu/ZrO2 based catalysts were evaluated by in situ facilities at BNL. AP-XPS and DRIFTS techniques were utilized to determine the adsorption strength and configurations of CO2 and key intermediates. The most important active intermediates in methanol production from CO2 conversion were identified. Pathway mechanisms, electronic and structural properties of catalysts were evaluated.

Abstract
In the last decade, the chemistry of carbon dioxide has drawn extensive attention because of its potential commercial interest and the utilization of carbon dioxide as a substrate for clean fuel production. CO2 recycling to produce methanol can be considered a catalytic system of high interest in industry, since methanol is a vital raw material for the petrochemical and chemical industries. In this regard, forming methanol by CO2 hydrogenation is one of the promising, effectual and economic techniques for utilization of CO2, and it can be a key to reducing atmospheric emissions and helping to satisfy a high energy demands. The purpose of this research is to improve the understanding of surface interactions on reactant-active sites in the CO2 conversion process to methanol synthesis over Cu-ZrO2-based catalysts. For this work, Cu/ZrO2 based catalysts were synthesized by a surfactant-assisted co-precipitation method using Pluronic (P-123) as a template and were evaluated under operando and in situ facilities at Brookhaven National Laboratory. Ambient pressure techniques, such as AP-XPS and Infrared Spectroscopy were utilized to determine the adsorption strength and configurations of CO2 and key intermediates. Furthermore, operando techniques, such as synchrotron-based XRD and X-ray absorption were employed to characterize the electronic and structural properties of catalysts under in situ conditions. In addition, two other groups of CuZnZr catalysts were evaluated by in situ AP-XPS and Infrared Spectroscopy techniques. Thus, it was identified as the most important active intermediates in methanol production from CO2 hydrogenation. Pathway mechanisms as well as the electronic and structural properties of catalysts focusing on increasing its selectivity were evaluated.

Parallel session topic: *Catalysts* **# C.1.4**

Gold Hybrid Catalyst for CO2 Conversion

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Keywords
CO2 conversion; Catalysis; Gold Catalyst

Impact statement
Disposing carbon dioxide in the atmosphere is no longer an option. Global warming is one of the most serious problems the humanity is facing, changing fauna, flora and the world as we now over the years. Thus, carbon capture and storage (CCS) and carbon capture and utilization (CCU) technologies are considered crucial for meeting CO2 emission reduction targets.

Highlights
CO2 emission is no longer a option. Carbon Capture and Utilization (CCU) is considered crucial for meeting CO2 emission reduction targets. Gold Hybrid Catalysts has been prepared in the present work. Au/TiO2 presented higher RWGS selectvity at low temperatures Au,Pd/SiO2 presented higher ethanol porduction than Pd/SiO2 and Au/SiO2

Abstract
Gold and palladium catalysts have been prepared to study the selectivity for CO2 hydrogenation to products of interest. At low temperatures, high selectivity for CO (RWGS), when compared to methanation was observed when Au/TiO2 and Pd/SiO2 were used. As the temperature increases, the Pd/SiO2 catalyst forms more methane than the gold or bimetallic catalysts. In the bimetallic catalyst, the C3 production increased, and ethanol was obtained by Au/SiO2 catalyst and the bimetallic catalyst. The increase in the carbon chain is interesting for the formation of products with higher added value.

Parallel session topic: *Optimization* **# C.2.1**

Adsorption-PCM multimaterial mixed Vessels

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Keywords
Phase Change Materials, Adsorption, Optimisation

Impact statement
Adsorption technology has many environmental and industrial applications, such as cooling, desalination, gas separation, storage and dehumidification. Therefore, these processes not only improve daily lives as they also have the potential to lower carbon footprint by recovering low-temperature waste heat sources.

Highlights
Modelling of adsorption vessel in finite elements; - Coupling between adsorption equations and phase change material equations; - Optimisation regarding the distribution of phase change material inside the vessel; - Experimental apparatus support.

Abstract
Numeric / Simulation The use of natural gas has become economically attractive for the industrial sector, and the form of its storage assumes an essential role in this process. The mechanism of mass transfer by adsorption is inserted in several areas of science and is already used for the storage of natural gas when applied to gas adsorption tanks. In parallel, phase change materials are present in latent heat storage applications and bring significant benefits in terms of thermal stability and thermal storage to volume ratio. Studies using phase change materials in adsorption tanks demonstrate improvements in the adsorption capacity of the tanks by improving the thermal behaviour of the set. Furthermore, geometry and position of the bodies belonging to the system influence the results; thereby signalling an opportunity to optimise the distribution of material inside the tank. The method of topological optimisation presents itself as an extremely generic tool for the distribution of material within a domain. The present study proposes to optimise the distribution of several combinations of phase change material and adsorbent inside an adsorbent vessel. The domain inside the vessel is considered to be a mixture of phase change material and adsorbent. Six conditions are analysed and compared to verify each scenario is most suitable for PCM insertion. Results show that the mixture PCM and adsorbent increase the amount of gas an adsorption vessel can deliver by the end of the discharging cycle. Experimental The kinetic study aims to observe the behaviour of the PCM and whether there is a difference in conductivity of the PCM according to their crystallisation kinetics, using a model based on transport phenomena and cold finger experiments. A cold finger PCM crystallisation model was developed using equations of heat transport phenomena and crystallisation concepts. The experiments were performed with commercial paraffin 120 / 125-6 (crystallisation temperature of 48 °C). The cold finger equipment was used, passing cooling water at 10 and 20 °C and melted paraffin at temperatures of approximately 53 and 58 °C, the four experiments lasting up to 30 min. The results indicate that there is good compatibility between the model and the experiments and that there is variation between the conductivity of the PCM and the crystallisation kinetics, which may interfere with the functioning of the PCM inserted in an ANG cylinder.

Parallel session topic: *Optimization* **# C.2.2**

Novel material model for topology optimisation of compressible fluids

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Keywords
Topology Optimisation, Compressible Flow Problems, Supersonic Separator

Impact statement
To the best of the authors knowledge, Topology Optimisation (TO) has only been applied to incompressible fluid flow problems. The development of a suitable material model for the compressible case will expand TO to a novel field of applications, and in particular can be used to generate optimized nozzle geometries for the supersonic separator.

Highlights
A novel material model is developed in order to use TO in inviscid compressible fluid problems
Governing equations solved using Least-Squares Finite Element Method
Computer program that uses only open source software

Abstract
The supersonic separator is a new compact and efficient technology for CO2 separation from Natural Gas with high CO2 fraction. It consists of a supersonic nozzle with a swirling flow. The cooling caused by the expansion of the flow leads to condensation of the CO2, which then moves to the outer portions of the nozzle due to centrifugal effects, where it can be collected. The use of computer simulations in the design of such devices have become essential, due to the flexibility in the analysis of different operation conditions, before the actual construction of the prototype, which lower the cost and avoid unnecessary experiments. One computational method that have been extensively used, in other fields of study, during the design project is the Topology Optimization (TO). The main advantage of TO is to obtain a non-intuitive optimized geometry for a given functional or metric of interest, even in the early stages of the project. TO have been successfully applied to different problems, such as structural analysis, thermal devices, among others. However, in fluid flow problems this methodology has been only applied to incompressible fluids. Thus, the main objective of this work is to implement a novel material model that can be used in TO applied to compressible fluid flow problems. As a preliminary work, the hypothesis of inviscid compressible fluid and the perfect gas assumption are considered. The Partial Differential Equations (PDEs) are solved using Least-Squares Finite Element Method (LSFEM) and implemented with the aid of the FEniCS library, an open-source software. The results of the proposed material model are verified in two different cases of a bidimensional nozzle, one with the presence of a normal shock and one without.

Parallel session topic: *Optimization* **# C.2.3**

Acoustic Inverse Problem by Using Topology Optimization

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Keywords
Acoustic Inverse Problem, Topology Optimization, Finite Element Method, Transient Analysis, Time-Harmonic Analysis

Impact statement
This work is part of the STMI project which aims at the development of numerical techniques and software for inverse problems with applications in seismic processing. Through implementation in high-level programming languages, a generic and systematic methodology for imaging inversion will be developed based on the Topology Optimization Method (TOM).

Highlights
The development of a methodology based on the Topology Optimization Method using a scaled material model - Finite Element analysis considering implicit time integration scheme and time-harmonic fields - The application of automatic differentiation tools for the adjoint problem - Different approaches to avoid the so-called "inverse crime" are analyzed

Abstract
Acoustic Tomography (AT) is referred to the inverse problem where unknown parameters of a given media of interest are estimated from precise measurements of acoustic propagation properties. In the geophysics field, seismic research is an important step in the production of oil and gas, either for the discovery of regions for prospecting or control of reserves in operation and, therefore, accurate solutions from the AT process can reduce the exploration and production costs. The main objective of the present work is to develop a generic and systematic methodology for solving the acoustic inverse problem based on the Topology Optimization Method (TOM), considering applications in both time-harmonic and transient regimes. The TOM is a method based on the distribution of the material in a fixed design domain combining optimization algorithms and numerical modeling techniques such as the finite element method (FEM) to minimize or maximize a cost function subject to inherent constraints to the problem. The literature review reveals that there is no application of TOM in AT problems, however, it has already been used in acoustic optimization problems which indicates a promising research topic to be explored. Compared to traditional methods, a TOM-based algorithm could provide better solutions by introducing the material model concept for the description of the properties of the media. In this work, the optimization problem is formulated to minimize a least-squares misfit function which takes into account the predicted and observed seismic shot records either in the time or frequency domains. A linear parametrization rule is employed to model the acoustic properties of the media considering nodal design variables. Automatic differentiation tools are employed for the adjoint problem and the optimization problem is solved using a quasi-Newton method with simple box constraints on the design variables. Preliminary numerical results considering strategies to avoid the so-called "inverse crime" are presented to verify the proposed methodology.

Parallel session topic: *Optimization* **# C.2.4**

Level-set method based on reaction-diffusion equation applied to acoustic (elastic) full-waveform inversion

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Keywords
full-waveform inversion; topology optimization; level-set; reaction-diffusion; finite element method

Impact statement
This research aims at developing a new proposal for solving the FWI problem with a topology optimization approach based on the level-set method. It should provide an efficient procedure to identify subsurface features, in association with high-performance computational systems. This procedure is a promising method for the identification of, for instance, salt formation and gas reservoirs.

Highlights
Solution of seismic FWI problems by means of the FE method and Topology Optimization concepts based on the Level-Set method; - Level-set approach using reaction-diffusion equation, making possible thoptimization without any initial information/guess about the topology to be identified (without initial holes); - Promising results by simple examples. Potential application in seismic exploration.

Abstract
Inverse methods are essential part in solving many engineering problems. Exploration geophysics benefits from the solution of inverse problems in the reconstruction of subsurface images. In this context, Full Waveform Inversion (FWI) has become an important technique to obtain high-resolution models based on data-sets recorded in seismograms. The main objective of such a method is to provide a description of subsurface constituents distribution (velocity model) by fitting synthetic and experimental data, respectively from numerical models and field survey. This method is naturally set as an optimization problem in which design variables have to be determined, and where several mathematical and numerical distinct approaches can be used. The current research focuses on the study and development of an optimization procedure to solve the FWI problem. Such a procedure is based on the Finite Element Method (FEM) and Topology Optimization (TO) concepts. In this context, the Level-Set (LS) method was chosen as a convenient technique to be investigated and applied, making possible to identify two-phase, or even multiple-phase media, as typically found in seismic exploration. A level-set function determines the material distribution implicitly by a (zero)-level curve. Then, a minimizing sequence is achieved by updating the level-set considering the gradient direction of the objective function. This is obtained by means of sensitivity analysis, which provides a level-set driven-velocity. By considering this driven-velocity and a reaction-diffusion partial differential equation, it is possible to update the level-set function, thereby allowing to update the slowness field of the acoustic (elastic) problem. The formulation for direct and adjoint problems in their continuous and discrete versions is presented, providing the basis for numerical implementation. Some examples are shown in order to evaluate the behavior and efficiency of the technique being proposed.

Parallel session topic: *Initiatives and Policies* **# C.3.1**

Creating an Energy Law Centre: RCGILex case

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Keywords
Energy Law, Energy Transition, RCGILex

Impact statement
RCGILex aims to organize the Brazilian and Paulista Natural Gas law service in a comprehensive perspective. The service is becoming a broad compilation of the Federal and state level regulations; along with comments from experts. RCGILex is a Law Centre, which is dedicate to understand the Energy transition under regulation in Brazil by lessons from international experience.

Highlights
Energy transition needs to be build according to national rules. Energy Law Centre is an important tool to instigate a solid debate. Analyzing the legal framework is key to collaborate to Energy transition. RCGILex became a tool to discuss and debate legal changes in natural gas. RCGILex is willing to reach out to other energy areas in order to better comprehend Energy transition.

Abstract
This project had the objective to describe how was the creation and development of a Legal Center of natural gas with the Brazilian federal and the state of São Paulo legislation, named RCGILex. During RCGILex construction, also we discussed the natural gas chain and some of its regulatory barriers. Related to the creation of the Legal Center, after doing a research and analysis of other sites of Legal Centers, especially the Canadian, we designed our own classifications in order to define the content of our Law Center. The project 21 planned to organize the Brazilian and Paulista Natural Gas Law Center. To do so, we studied methodologies of classification of different Legal Centers and then we started to design our own repository. Our motivation is to contribute to the regulation of natural gas in Brazil. RCGILex is linked to Project 21 from RCGI - Research Centre for Gas Innovation . Under this research, we developed a Gas law Center, RCGILex (http://rcgilex.com.br/) and a tool to search law and its comments (https://app.rcgilex.com.br/). This Project was developed within RCGI, which is "a world center for advanced studies of the sustainable use of natural gas, biogas, hydrogen and management, transport, storage and usage of CO2. The center, based at the University of São Paulo, is the result of FAPESP partnerships in support of high-level scientific research for the development of the energy sector. Its activities are based on three pillars: research, innovation and dissemination of knowledge" (RCGI, 2019). Professor Dr. Julio Meneghini (https://www.rcgi.poli.usp.br/professor-julio-meneghini/) is Scientific Director from RCGI (https://www.rcgi.poli.usp.br/). In addition, we highlight that the RCGI is grateful to the generous support of the founder sponsors: FAPESP and Shell (RCGI, 2019). We had finance from RCGI, which contemplates our research team with scholarships from University of Sao Paulo Foundation (FUSP). In addition, RCGI contracts S-SYS Company in order to develop the legislation tool search. Project 21 belongs to ENERGY POLICIES AND ECONOMICS PROGRAMME coordinated by Prof. Dr. Edmilson Moutinho dos Santos.

Parallel session topic: *Initiatives and Policies* **# C.3.2**

Spatially-resolved urban energy systems model to study decarbonisation pathways for energy services in Sao Paulo

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Keywords
Energy systems modelling; spatially-resolved; decarbonisation

Impact statement
One of the key barriers to further penetration of gas in Brazil is the lack of transmission and distribution infrastructure. This work addresses this issue by implementing a spatially resolved optimisation model that finds the most cost effective infrastructure development paths, trading off cost and performance across key energy vectors while meeting decarbonisation targets.

Highlights
Spatially-resolved urban energy systems model
Model supplies energy demands for heating, cooling, electricity, and transport
Model implemented to study decarbonisation pathways in Sao Paulo
Decarbonisation scenarios include electrification of heat and transport
High penetration of district cooling networks in high linear cooling density zones

Abstract
This work presents a spatially-resolved optimisation model for finding cost effective technology pathways for decarbonising energy services in urban areas, considering heating and hot water, cooling, electric appliances, and transport demands. The model trades-off the costs of network infrastructure, end-use technologies, and energy supply options. It was implemented for a case study consisting of six scenarios in the city of Sao Paulo, from which spatial and temporal demand profiles were obtained. Results showed that district cooling is cost-effective in the highest linear cooling density zones, with full penetration in zones with over 1100 kWh/m by 2050. This threshold diminishes as tighter carbon constraints are imposed. Heating is electrified in all scenarios, with electric boilers being the main technology for the domestic sector, and air-source heat pumps with some gas boilers supplying the commercial sector. In carbon emissions constrained scenarios, different penetrations of combined heat and power and hydrogen boilers appear in the domestic sector energy mix, and ground-source heat pumps in the commercial sector. Finally, in the transport sector ethanol replaces gasoline, diesel and CNG cars, CNG buses replace diesel and electric buses, and diesel continues to be the dominant technology for lorries. In carbon constrained scenarios, higher penetrations of electric cars and buses are obtained, while no change is observed for lorries.

Parallel session topic: *Initiatives and Policies* **# C.3.3**

The Brazilian energy transition pathways: an emerging field of research

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Keywords
Energy Transition; Socio-Technical Transition; Emerging Technologies

Impact statement
The socio-technical systems offer undergo incremental rather than radical changes. On a world scale, there is not a single process of energy transition. Nations are in different stages of maturity, seeking their own paths of energy transition. Delivering pathways toward low-carbon industry (mainly oil industry) such as the implementation of Carbon Capture and Storage in Brazil.

Highlights
(1) Energy transition is redefining directions in an environment with high uncertainties. It is therefore a matter of making choices whose foundation requires long, medium- and short-term planning. (2) Challenges of the implementation of Carbon Capture and Storage in Brazil by looking at the socio-technical transition.

Abstract
The concept of energy transition has received increasing attention over the past 20 years, and currently, connected with to concepts such as socio-technical, have underpinned and demonstrate paths to a low carbon transition. To understand the socio-technical transition is a set of processes that occasion to an important change in socio-technical systems (technological, material, organizational, institutional, political, economic, and socio-cultural). Therefore, applying the socio-technical transition (multi-level perspectives) help us to discuss what the possibilities and urgencies, such as global warming and reduction in CO2 emissions, to a sustainable energy transition in a world that is reinventing itself at incredible speed searching for clean and renewable energies sources. The aim of this work focus on the network of stakeholders and the conditions needed for implementing Carbon Capture and Storage in Brazil by analyzing at the socio-technical transition. Base on that, it is necessary to review the situations where implementation was realized (e.g., Norway, United State for Enhanced Oil Recovery) and what may be needed in Brazil in the future in comparison. It does so by examining the environmental risks, the discourses between and networks of actors involved in this process and the investment and financial support from public and private stakeholders. Finally, actions to limit global warming to 1.5°C with no or limited overshoot have been required an acceleration to a low carbon system, including an effective contribution of the emerging technologies such as Carbon Capture and Storage. Being necessary, Research & Development projects that understand the entire chain of an emerging technology such as Carbon Capture and Storage, addressing and answering to the challenges for a sustainable transition.

Parallel session topic: *Initiatives and Policies* **# C.3.4**

Innovative Actions of the Research Centre for Gas Innovation building the path towards Sustainability Goals in Brazil

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Keywords
Triple Helix Innovation Model, Sustainable Development Goals (SDG), Agenda 2030 in Brazil

Impact statement
This work presents the main contributions of a triple helix innovation model, represented by the RCGI, towards the Sustainable Development Goals (SDG) of the United Nations and the Agenda 2030. The RCGI projects were analysed in order to comprehend the main results and their impact to support the goals. The study shows important contributions to at least 11 of the 17 SDGs presently.

Highlights
RCGI is proactively contributing to the Sustainable Development Goals.
The triple helix innovation model is producing positive results towards Agenda 2030 in Brazil.
Multidisciplinary groups are working together to provide solutions for the energy transition.
Innovation requires a broad approach that encompasses technical, economic, environmental and social aspects.

Abstract
This proposal describes actions connected with global sustainability goals implemented through the Research Centre for Gas Innovation (RCGI). RCGI's strategic vision, the research and the triple helix innovation model were detailed, considering the relationship between university (University of São Paulo), company (Shell) and government (represented by FAPESP funding agency), in the technological, environmental, social and economic areas. The Centre works by integrating its projects with the Sustainable Development Goals (SDGs), using these as a basis towards monitoring to follow the roadmap of the "Brazilian Agenda 2030 for Sustainable Development". RCGI is currently devoting its research to analysing the potential use of natural gas, biogas and hydrogen, and applying technologies to mitigate CO2 emissions and other greenhouse gases in order to provide a more sustainable future, accounting for innovations mainly in the field of cleaner and more sustainable energy, as well as positive actions to combat climate change.

Parallel session topic: *Gas Conversion* **# D.1.1**

Microbial Production of Polyhydroxybutyrate (PHB) from Methane

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Keywords
bioplastics;
polyhydroxyalkanoates;
methane mitigation

Impact statement
Methane causes harmful effects to several ecosystems because of its GWP 28 times higher than CO2. The unrestrained production of plastics worldwide coupled to its inappropriate disposal is another environmental issue of growing concern which intensifies the necessity of their remediation. This project aims at solving both problems at once producing biodegradable polymers using methane as feedstock

Highlights
Copper supplementation increased PHB production by 900%
Decrease in PHB production time in one third
Calibration curve assembling for conversion factors calculation
Algae and bacteria co-culture effects evaluation over PHB production

Abstract
Methane is the second most important greenhouse gas, presenting a global warming potential 28 times higher than CO2. It implies that methane is much more effective at trapping heat in the atmosphere, causing harmful effects to several ecosystems. In addition, methane emissions are increasing 10 ppb per year, making its mitigation necessary. On the other side, petro derivative plastics also represent a major threat to several ecosystems, especially when considered its large worldwide production and persistence in the environment due to their non-biodegradability. An alternative to solve both problems could be producing biodegradable plastics using methane as feedstock. Methanotrophs are a group of bacteria present in the environment that are capable of methane usage as carbon source, which results in natural accumulation of polyhydroxybutyrate (PHB) inside their cells as energy reserve granules. PHB is a biodegradable polymer with characteristics similar to those of polypropylene (PP), the most used type of plastic worldwide. However, PHB's production price is still very high and inhibits its entrance into the market, but the use of methane as feedstock could help decrease it and make it feasible. The main goal of this project is to find these microorganisms in the environment and stimulate PHB production under methane atmosphere. Four consortia obtained from different mangrove areas were tested for PHB production. Methane atmosphere in air (1:1.5 CH4/O2 molar) was used to ensure complete methane oxidation. Experiments were performed in 250 mL shake flasks containing 50 mL NMS medium culture under 28ºC and 180 rpm for 12 days. Atmosphere was replenished every 48 hours. Copper was supplemented at 10 mM concentration at the final medium composition to evaluate if methane uptake would increase. The best results of PHB production were obtained by a consortium (1SED) collected from a sediment sample of Guarujá's mangrove. In the presence of 10 mM of copper, PHB production reached 0,2 g.L-1 after 4 days in N-free NMS, representing accumulation of 20% in cell dry weight. PHB characterization and quantification were performed by GC-FID. This consortium was also co-cultured with the algae Parachlorella kessleri in 5% CO2 in order to investigate its effect on PHB accumulation. At the moment a calibration curve is being arranged to enable the calculation of product conversion factors.

Parallel session topic: *Gas Conversion* **# D.1.2**

Extracellular carotenoid production from microalgae under increased CO2 concentrations

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Keywords
carotenoid, microalgae, photobioreactor

Impact statement
Carbon dioxide fixation by microalgae represents a scientific and economic interesting approach for CO2 mitigation, since they selectively use this gas to produce high value bioproducts difficult to be obtained by chemical routes, such as long chain polyunsaturated fatty acids (omega-3 and omega-6) and carotenoids, with nutritional and pharmaceutical applications.

Highlights
Selected microalgae were able to grow using gas streams with up to 30% CO2
Relatively simple production of high value bioproducts using CO2 as only carbon source and mild conditions in photobioreactor
To our knowledge, the first reported microalga to produce an extracellular carotenoid as bioproduct, reducing the costs of chemical extraction and increasing the sustainability of the process

Abstract
Carbon dioxide fixation by microalgae represents a scientific and economic interesting approach for CO2 mitigation, since they use this gas to produce high value bioproducts difficult to be obtained by chemical routes. Fast-growing and high CO2-tolerant microalgae were pre-selected under 30% CO2 from water and sediment samples, isolated using appropriate techniques, identified via molecular biology and evaluated with cultivations in shake flasks under CO2 concentrations from 5% to 30%. Parachlorella kessleri presented the highest biomass production and growth velocities under all tested CO2 conditions, besides producing an extracellular red pigment with antioxidant activity. Some of the antioxidants reported in microalgae are: neoxanthin, violaxanthin, lutein, zeaxanthin, ß-carotene, anteraxanthin, astaxanthin and canthaxanthin. Among them, astaxanthin is the highest-value carotenoid produced from microalgae that has achieved commercial success. The production of antioxidants in some cases occurs when microalgae are subjected to stress, which can be high CO2 levels. This work evaluated extracelullar carotenoid production from Parachlorella kessleri in stirred tank photobioreactor (2 L of working volume), cultivated under 5%, 15% and 30% CO2. In the 10th day of cultivation, CO2 supply was interrupted until the end (14th day), which probably causes a stress for microalgae cells and is imperative condition to make them produce the antioxidant. Under 5% and 15% CO2, the reddish carotenoid production was observed, with higher yields under 15% CO2. On the other hand, 30% CO2 did not seem to achieve sufficient condition to produce the reddish pigment, producing a yellowish one. Research is being conducted on purification methods using High Performance Liquid Chromatography (HPLC) and chemical characterization of both pigments by UV-Vis absorption, Mass Spectroscopy (MS) fragmentation and Nuclear Magnetic Resonance (NMR) to elucidate their chemical structure. Results so far have pointed to a carotenoid with molecular weight 569 g/mol, corresponding to zeaxanthin or lutein in the microalgae metabolism, although further results are necessary to confirm this hypothesis. This step is crucial to improve the production process to maximize carotenoid production.

Parallel session topic: *Gas Conversion* **# D.1.3**

Achieving high selectivity towards CO from reverse water-gas shift reaction on classical Ni/SiO2 catalysts

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Keywords
CO2 abatement, nickel, selectivity

Impact statement
The Reverse Water-Gas Shift Reaction (RWGS) is a handful way to produce syngas from CO2. Ni catalysts are important for this reaction; however, they are also active for CO2–CO hydrogenation to CH4, which is undesirable. In this work, we propose a simple procedure in classical Ni catalysts to improve its selectivity towards CO and suppress the CH4 formation.

Highlights
The properties of the catalysts were exhaustively studied by XPS, FTIR and XAS, besides the catalytic tests. After this ageing step under CO2+H2 atmosphere at high temperatures, a poisoning of the active sites for CH4 formation occurs via enhancement of carbon species. These species block mainly the sites that can bond CO strongly, increasing CH4 formation.

Abstract
The reverse water-gas shift (RWGS) can be understood as a model reaction to probe the properties of heterogeneous catalysts, besides it can be a way to convert CO2, a greenhouse gas, to CO that can be further used in Fisher-Tropsch processes. Selectivity is an important issue on Ni catalysts, which can favor the complete hydrogenation of CO2/CO to CH4. The selectivity can be governed by nanoparticle structure. Although small nanoparticles tend to avoid the complete hydrogenation, the stability of such catalysts can be an important issue. Herein we report classical Ni/SiO2 impregnated catalysts under RWGS conditions. The catalysts are active for CO2-CO hydrogenation to CH4 at low temperatures, but after thermal treatments under different atmospheres, the CH4 formation is suppressed. This can be related to poisoning of the most active sites for CH4 formation, as probed by different approaches. A carbon structure on the top of Ni nanoparticle is the key to addressing selectivity towards RWGS reaction, which might be a very important finding in the CO2 conversion to chemicals.

Parallel session topic: *Gas Conversion* **# D.1.4**

SYSTEMATIC SCREENING OF IONIC LIQUIDS FOR HYDROGENATION OF CO2 TO FORMIC ACID AND METHANOL

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Keywords
Ionic liquids; Formic acid; CO2 hydrogenation

Impact statement
A significant benefit of ionic liquids as the solvent in hydrogenation reactions is the ability to fine tune the properties of the solvent by altering the structure, catalyst immobilization and activating the CO2, consequently leading to reduction in Gibbs energy of formation of formic acid.

Highlights
Screening strategy based on phase equilibria calculation, physical property prediction, and process simulation Independent analysis on mole and mass were performed. Three promising ionic liquid candidates with excellent properties that satisfy both the mole and mass-based criteria. The three candidates can be applied to promote hydrogenation of CO2 to formic acid.

Abstract
The use of carbon dioxide as a raw material for chemical synthesis constitutes an ecologically and economically useful addition to existing carbon sources. In order to convert the thermodynamically stable and relatively unreactive CO2 molecule into the desired product efficiently, suitable reaction conditions and activation mechanisms must be found. Ionic liquids (ILs) may be viewed as a new and remarkable class of solvents. One significant benefit of ionic liquids as the solvent in hydrogenation reactions is the ability to fine tune the properties of the solvent by altering the structure, catalyst immobilization and activating the CO2, consequently leading to reduction in the Gibbs free energy of formic acid. A systematic strategy for the selection of ionic liquids as solvent for the hydrogenation of CO2 combining phase equilibria calculation, physical property prediction, and process simulation is presented. The liquid-liquid equilibrium of the reactants and different ionic liquids are predicted with the conductor-like screening model (COSMO), which was performed independently both in mole and mass-based. Consequently, the ionic liquids are pre-screened with higher distribution coefficient, selectivity and solvent loss (mass and mole). COSMO was also employed to estimate the important physical properties of the pre-screened ILs and further suggest candidates meeting certain physical property constraints. Afterward, qualitative and quantitative analysis of the final candidates of ILs impact on the environment based on octanol/water partition coefficient. Finally, the separation performance of the top IL candidates in a continuous process is analyzed by Aspen Plus to finally identify process-based optimal solvents. The three most promising ionic liquid (Anilinum nitrite, 1-methylimidazolium nitrite and 1-pentyl-imidazolium nitrite) for this process are consequently determined.

Parallel session topic: *CO2 in salt caverns* **# D.2.1**

Conceptual design of offshore salt caverns for CCS

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Keywords
Offshore salt caverns, subsea system, flow assurance.

Impact statement
No offshore operations in salt caverns were identified, in shallow or deep water. There are no operations of CO2 confinement in salt caverns. The offshore salt cavern CCS project is a combination of two areas: onshore salt cavern natural gas storage and deep water oil & gas production

Highlights
Conceptual design of offshore salt cavern as CCS system
Storage of CO2 rich stream
Riser and flowline defined by coupled subsea and flow assurance models
Subsea arrangement considers risers in free standing or lazy wave.

Abstract
The use of salt caverns for confining hydrocarbons has a long history around the world. The world's largest crude oil reserve is stored in 62 salt caverns opened by solution mining in salt domes distributed in different USA locations. The offshore salt cavern CCS project is a combination of two areas: onshore salt cavern natural gas storage and deep water oil & gas production. Typical technologies from such areas are applied, such as 3D sonar scan to monitor cavern shape, pre-salt well design, stability analysis through geomechanical simulation, and mechanical integrity tests (MIT). At least two uses of offshore salt caverns are foreseen: as CCS system to confine a stream with high CO2 content, and as gravitational separators to generate a hydrocarbon rich gas stream that can be monetized. An experimental system is proposed to investigate and validate both concepts. For CCS to be successful, three fundamental conditions are required: Capacity, injectivity, and confinement. The CCS technological solution considers up to five main elements: a drilling rig, a floating unit dedicated to solution mining, a brownfield FPSO that injects the CO2 rich stream, a flow system comprised of a subsea arrangement and one or more wells, and salt caverns opened by solution mining. The subsea conceptual design of the offshore salt cavern CCS system comprised the following phases: salt cavern dissolution (solution mining), brine substitution and pressurization. Subsea and flow assurance models were coupled to achieve optimum configurations in terms of power consumption and riser/flowline weight, while maintaining an acceptable safety level.

Parallel session topic: *CO2 in salt caverns* **# D.2.2**

Strategic Plan for Constructing Ultradeep Offshore Caverns for CO2 Confinement in the Brazilian Pre-Salt Oil Fields

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Keywords
Salt Cavern, Strategic Planning, Integer Programming Model

Impact statement
This usage of salt caverns built within the salt-layer for CO2 confinement has been considered by players from the oil & gas industry. This research proposes a strategic plan for supporting the implementations of such caverns by optimizing their construction schedule while deciding on the level of the critical resources and of the construction sequence.

Highlights
CCS is addressed in the context of gas production from Brazilian pre-salt oil fields. Salt caverns built within the pre-salt layer are considered for CO2 storage. A strategic plan is proposed to select the caverns to build and when to build. The plan includes deciding on the level of the critical resources. A mixed integer mathematical programming model is proposed and solved.

Abstract
The production of natural gas from the pre-salt oil fields in the Brazilian continental shelf has many technological challenges, among which the destination of the CO2 content present in the natural gas. A novel alternative has been investigated and consists of using ultra-deep offshore caverns as depots, built within the salt layer, to receive the CO2 originated at one or more production units. The building process requires specialized resources, including drilling rigs, special purpose construction vessels and subsea pumps. This paper proposes a mathematical model for supporting a construction plan for building caverns in Lula Field, Brazil. Among a list of candidate sites for opening caverns, it should be decided which caverns to build, their sizes and leaching speeds, and when to begin their construction. By taking as a constraint the CO2 storage capacity to be delivered within a given planning horizon, the plan encompasses the definition of each resource level with the objective of minimizing the total capital expenditure. This problem is modeled as a mixed integer program and solved using commercial optimization software.

Parallel session topic: *CO2 in salt caverns* **# D.2.3**

The screening and scoping of Environmental Impact Assessment of CO2 Storage in Brazil

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Keywords
Screening; Scoping; Environmental Impact Assessment; Storage

Impact statement
There are still no specific Environmental Impact Assessment frameworks for the various phases of Carbon Capture and Storage in Brazil. Therefore, describing the criteria of these phases will contribute to the elaboration of a specific framework to the country.

Highlights
To describe criteria for screening and scoping phases of the Environmental Impact Assessment to CO2 storage.

Abstract
The aim of this paper is to analyze criteria for the development of screening and scoping phases of the Environmental Impact Assessment for CO2 storage. The Screening phase of the Environmental Impact Assessment contribute to identify whether the proposed project is potentially or effectively causing significant environmental degradation and, accordingly, address which studies and procedures for its Environmental Licensing will be. In this case, the research identifies criteria of environmental vulnerability applied of offshore areas, mainly Pre-Salt area, where the screening methodology was applied by Brazilian Institute of Environment and Renewable Natural Resources (Instituto Brasileiro do Meio Ambiente e dos Recursos Naturais Renováveis IBAMA) in the exploration of oil in the country. On the other hand, we analyze what are the necessary steps for scoping phase of Environmental Impact Assessment for CO2 storage, considering that Brazil already has some on and off shore CO2 storage experiences (CBM/ECBM Pilot Site in Rio Grande do Sul state and Tupi Pilot Site in Santos basin), but all characterized as enhanced storage and therefore included within production projects already licensed and evaluated. That is, in none of these cases was the storage project the object of a single Environmental Impact Assessment process, which demonstrates the relevance of this work by analyzing criteria for processes that consider CO2 storage as a project to be licensed individually.

Parallel session topic: *CO2 in salt caverns* **# D.2.4**

Offshore Salt Cavern Case and its Legal Aspects

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Keywords
Legal Aspects of CCS; Brazilian PreSalt Area; Salt Cavern

Impact statement
Through a case study of the salt cavern for the Brazilian Pre-Salt region, this paper addressed the relevance of the implementation of CCS activities to the hydrocarbon production of CO2 and EOR and its legal aspects as Property Rights, Environmental Standarts and Licensing and Public Participation.

Highlights
Carbon capture and storage (CCS) is a technology tool to help countries to meet their CO2 emissions targets by 2030.
Salt Cave case can help to implement CCS activities linked to hydrocarbon production and EOR.
It is fundamental to address legal aspects as property rights, environmental stardarts, environmental licensing and public participation.

Abstract
Carbon capture and storage (CCS) appears as a technology tool to help countries to get their CO2 emissions lower and accomplished targets by 2030. As any humankind activities, CCS must follow legal constraints. Those are important issues to be considered in order to put carbon capture and storage projects in place. Therefore, this paper aims to describe and analyze the legal and environmental aspects about CCS in Brazil. Our methodology includes comparative law method and a case study that is Salt Cave Offshore located in Pre-Salt area. First, we must understand propriety rights, including operational permitting and others issues; after considering the cycle of life's projects, its development and appropriated managed, control and closing; finally, environmental and public participation during project running life. Our intent is to contribute to Brazilian discussion on CCS legal framework in order to avoid conflicts and draw answers which law should be applied.

Parallel session topic: *Policies and Regulation 2* **# D.3.1**

Incentives Impact on the Diffusion of Alternative Fuel Vehicles in Brazil

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Keywords

Alternative fuel vehicles; Tax impacts; Diffusion of technologies model

Impact statement

Our article uses an innovative diffusion model that allows us to detect the impact of marketing variables over successive technological generations of alternative fuel vehicles in Brazil. We observed how the loss of consumer confidence contributed to the failure of the ethanol technology during the 1990s, as well as, the factors that contributed to the success of the flex technology.

Highlights

Tax reduction has incentivised the diffusion of alternative fuel vehicle in Brazil. Successful new technological generations increase market potential as a whole. Ethanol technology was boosted by innovation tendency but hindered by word-of-mouth. Flex vehicles diffusion is supported and maintained by word-of-mouth.

Abstract

The transportation sector is responsible for nearly a quarter of greenhouse gases emissions (GHG); thus, incisive policies are necessary to mitigate the sector's effect on climate change. Promoting alternative fuel vehicles (AFV) is an essential strategy to reduce GHG emissions in the short term. Here, we study the effects of governmental incentives on the diffusion of ethanol and flex-fuel vehicle technologies in Brazil. We use a multi-generation diffusion model which assumes that new technologies introduce fresh market potential for adopters as well as upgraders from established technologies. Our analysis indicates that tax rates affected the adoption of both gasoline and ethanol technology, but for flex vehicles, the effect of taxation is not significant. The effect of fuel price shocks during the 1990s meant that the introduction of ethanol technology made no significant impact on market potential and a negative word-of-mouth effect contributed to the technology's failure. In contrast, the introduction of flex technology led to almost a doubling of total market potential. As policy suggestions, we emphasise the importance of tax reduction in addition to promoting versatile technologies, which insulate consumers against price fluctuations.

Parallel session topic: *Policies and Regulation 3* **# D.3.2**

Addressing climate change on standards – An ISO/TMB guideline

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Keywords
standards; guidance; climate change

Impact statement
This research reports the development of ISO Guide 84 "Guidelines for addressing climate change in standards". By applying this guide on creating or revising standards, users will be better prepared to tackle climate change mitigation and/or adaptation and understand that their organizations have possibilities to approach to these challenges.

Highlights
Climate change is acknowledged as a foremost challenge with regards to the goal of sustainable development. International standards that take into consideration climate change adaptation and/or mitigation can contribute to the achievement of sustainability. Standard writers are encouraged in the creation or revision of standards to consider climate change topics in their activity at all stages.

Abstract
Climate change is affecting many parts of the globe, including its impacts, risks, and opportunities from changing weather patterns, increasing sea level, and more extreme weather events. The possible impacts of such climate-related effects include disrupting various environmental, social, and economic systems within several nations, affecting communities and organizations, as well as individuals, and the most expected to be impacted by are the poorest and most vulnerable people. Action is essential, involving both climate change mitigation and adaptation, to reduce the implications of climate change, while also contributing to the reduction in the rate of increase of the global average surface temperature. The scope, need, and opportunities for action on climate change are vast towards this complex perspective. International standards that take into consideration aspects of adaptation and/or mitigation of climate change can contribute to sustainable development. Standard writers are encouraged in the creation or revision of standards to consider climate change topics in their activity at all stages. When standards writers tackle climate change in existing or new standards, the outcome can be improved awareness among the user community about climate change issues across distinct economic sectors. This research reports the development of ISO Guide 84, entitled "Guidelines for addressing climate change in standards", an ongoing work conducted by the Task Force on Climate Change Coordination (CCC TF) of ISO Technical Management Board (ISO TMB). By applying this guide, standard users will be better prepared to tackle climate change mitigation and/or adaptation in ways not generally anticipated and will understand that their organizations have possibilities to approach to these challenges in ways not initially perceived.

Parallel session topic: *Policies and Regulation 4* **# D.3.3**

CCS international standardization – threats and opportunities

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Keywords
CCS, standards, geological storage

Impact statement
The development of standardization on CCS has been advancing since 2011, including CO2 capture, transport to a final location, storage, closure and preparation for long-term administration. Methodologies are being agreed to allow their application to advance globally, setting the stage for CCS regulatory challenges around the world. Following this movement represents challenges and opportunities

Highlights
The ongoing work on CCS is using different guidelines and standards in its methodological considerations. Setting specific standards can be considered a benefit to technology proponents, regulators and the public sector as it can provide assurances that CCS projects follow internationally accepted practices for safety and environmental integrity.

Abstract
In 2011, within the framework of the International Organization for Standardization (ISO), the ISO/TC 265 Carbon dioxide capture, transportation and geological storage Technical Committee was set up to develop international technical standards dealing with the full life of a Carbon Capture & Storage (CCS), including CCS-specific technologies, terminology, environmental considerations, risk management, Greenhouse Gases (GHG) quantification and verification, health and safety and other CCS-related activities. Developing international standardization is a priority approach to promoting CCS because it builds on the growing international knowledge and experience in this field of knowledge, as well as recognizing technologies and projects that can reliably cross borders and jurisdictions through the standardization of concepts, methodologies and technologies used, benefiting the world in mitigating actions to combat climate change. This preliminary study deals with the survey of the development situation of the international standardization of CCS within the scope of ISO TC 265 and analyzes the possibility of capturing knowledge and experiences in the field of standardization of processes and associated technologies. From this initial survey, the research is dedicated to evaluating the necessary developments to establish an infrastructure (framework) that allows interacting with the development of international standardization, through the representation of countries and organizations. It seeks to identify the priority themes in the international sphere where Brazilian influence is desirable to take into account the relevant and particular aspects in the Brazilian oil and gas production scenario, acting effectively in the construction of international technical standards; and to establish the development of Brazilian standards that may serve to disseminate knowledge and standardization of CCS-related issues locally, while taking into account broader regulatory aspects that address the issue in Brazil.

Parallel session topic: *Policies and Regulation 5* **# D.3.4**

Regulatory Sandboxes to Safely Apply Blockchain Technology in the Energy Sector

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Keywords
Blockchain, Regulation, Sandboxes

Impact statement
Regulatory sandboxes are safe environments that loosen power sector regulations to permit experimentation before applications can turn mainstream. This way, it is possible for blockchain ventures to set up small-scale demonstration projects - a crucial step to turn blockchain's potential into reality.

Highlights
The first stage of blockchain for energy was the maturing of the technology, that faded initial hype away and led many corporate players to develop serious projects, On earlier stages, blockchain in the energy sector was associated almost exclusively with peer-to-peer energy. Now, new models have evolved and that is leading us to a second stage: regulation.

Abstract
The global energy sector is facing multiple concurrent disruptions that are fundamentally transforming electricity markets, usually expressed by the 3Ds: digitalization, decarbonization and decentralization. But there is one technology in particular that was born in the financial sector and is moving quickly and gaining momentum in the energy space as a solution for such disruption: blockchain. The possibilities we can seize with blockchain are immense: a way to make a decentralized electricity grid more secure against cyberattack by eliminating vulnerable, centralized single points of failure; a way for millions—and eventually, billions—of DERs to connect, verify, and transact with one another; a way for the green attributes associated with renewable energy to be tracked and traded with unprecedented levels of transparency and automation, streamlining costs and enabling greater market participation; a way for EVs to become cooperative and interactive grid assets, rather than "dumb" sources of spiking grid demand that exceed circuit capacities. (Bronski, 2019) The first stage of blockchain for energy was the maturing of the technology, that faded initial hype away and led many corporate players to develop serious projects, such as PJM in the United States, Iberdrola in Spain, SP Group in Singapore, and PTT in Thailand. One crucial step was for that was the evolution of business models, as on earlier stages, blockchain in the energy sector was associated almost exclusively with peer-to-peer energy. Now, new models have evolved around flexibility trading, renewable energy certificates (RECs), transactive grid and electric mobility. That is leading us to a second stage: regulation. Historically, the power sector has been highly regulated for very good reasons, such as protecting the customer, increasing competition and transparency, avoiding monopoly and oligopoly. But while such rules create protection to the final customer from bad corporate behavior, it also creates hurdles for innovation, since the small players have to follow the same rules as the giants. The objective of this research is to explore regulatory sandboxes that loosen power sector regulations to permit experimentation in a safe environment before applications can turn mainstream. This way, it is possible for blockchain ventures to set up small-scale demonstration projects - a crucial step to turn blockchain's potential into reality.

ABSTRACTS OF POSTER SESSIONS

Poster session **# P.01**

Mitigation of Methane Emission on ICE's: preliminary results

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Keywords
Dual fuel; prechamber; optical access internal combustion engine

Impact statement
Natural gas is a promising alternative fuel as it is affordable, available worldwide, has high knock resistance and low carbon content. The major drawback is its Global Warming Potential since methane is estimated to have a GWP of 28-36 over 100 years (CO2 is assigned as 1), which means that even small amounts of methane released in to the atmosphere are harmful to the environment.

Highlights
The optical access engine was commissioned. First CFD simulations of the engine were done. First images from methane combustion ignited by diesel pilot were acquired by means of natural luminescence (NL). Shadowgraph images for the methane jet in the prechamber were taken and the constant volume combustion chamber simulation was updated to predict the mixture formation inside the prechamber.

Abstract
Natural gas is a promising alternative fuel as it is affordable, available worldwide, has high knock resistance and low carbon content, however its Global Warming Potential is estimated as 28-36 times the CO2 over 100 years, which means that even small amounts of methane released in to the atmosphere at any stage in the transportation system or thermo-power plants may offset the benefits of CO2 emission reduction. Several papers show the trend of using fuel-lean combustion strategies, which yield lower in-cylinder temperature reducing the NOx emissions and heat losses, improving the thermodynamic efficiency. Fuel lean combustion also mitigates knock and hence enable high load operation. However, the lean limit is determined by the capability of the ignition system to reliably ignite the fuel-lean mixture. To overcome this limitation, alternative ignition strategies like laser induced ignition, diesel pilot injection and pre-chamber type ignition devices have been proposed in the literature. Comparing these alternative methods, a pre-chamber ignition system offers a more simplified solution since it requires minimum or no engine modifications and is structurally less complex. It can also be considered more advantageous from the environmental perspective since the pre-chamber makes it possible to run the engine solely on natural gas. In this research, the pre-chamber ignition system and the diesel pilot injection were studied by means of both experimental and numerical perspectives. Shadowgraph images for methane jet in the pre-chamber without bottom part to establish the spark time to ignite the methane-air mixture were taken. The probable spark times for ignition found experimentally were in agreement with CFD simulation. However, the gas mixture just ignited, but could not propagate away from ignition, due to the lack of oxygen and low temperature of the methane jet. Therefore, the air pressure will increase in the constant volume combustion chamber for the next experiments. First images from methane combustion ignited by diesel pilot in the optical engine were acquired. The natural luminescence (NL) images showed the combustion rotates clockwise for the majority of the cycles observed and for some of them the flame propagating inward from piston periphery towards the center was visualized. New NL images will be taken in order to better check the combustion quality and characteristics. CFD simulation results are compared to experimental data obtained.

Poster session **# P.02**

Optimization based on the adjoint method for natural gas storage systems

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Keywords
Optimization, Adjoint, CFD

Impact statement
The Adsorbed Natural Gas technology (ANG) has become an attractive alternative for storage systems. To a reasonable extent, the method provides a means of storing gas at substantially higher concentrations than what can be achieved with simple compression (CNG) at comparable pressures. Also, the method could be applied to study large storage systems focused in carbon dioxide capture.

Highlights
Complete Optmization algorithm based on Adjoint Method. Inverse design and optimization methods. Adjoint Method contour problem. Non Geometric sensitivities for operational conditions. Phenomena of Adsorption applied in Natural Gas or Carbon Dioxide.

Abstract
In the past few years, the development of inverse design and optimization methods has opened up new possibilities. The adjoint method is of great significance in that context, since it permits high fidelity to flow-physics at comparatively low computational costs. The present work focuses on adsorbed gas storage systems. Its contribution is the development of an alternative approach to the adjoint contour problem, which ensures that the latter is as well--posed as the physical problem, itself. This approach proves to be fully consistent with Cacuci's methodology of computing sensitivity derivatives, which enables us to extend their scope. It allows for the evaluation of sensitivities with respect to parameters other than those pertaining to geometry, i.e. to those that control the system operation. The main goal of this work is to obtain and validate a basic structure of an optimization loop algorithm (OLA) based on Adjoint Method applied in Adsorption Natural Gas Storage Systems.

Poster session **# P.03**

Fuel Cell Dynamic Model for Hybrid Vessel Power System

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Keywords
Fuel cell, dynamic model, hybrid power system

Impact statement
The present project aims to develop a fuel cell system dynamic model and use it as an alternative electrical energy source in an already developed Platform Support Vessel (PSV) hybrid power system dynamic model. The ship dynamic model has been used to access performance parameters such as fuel and energy consumption, emissions and power system components efficiency during various ship missions.

Highlights
Fuel cell dynamic model development. Alternative energy source for hybrid power system. Incorporation to a Platform Support Vessel (PSV) dynamic model. Simulations using Numerical Offshore Tank simulators (TPN).

Abstract
With the crescent relevance given to environmental issues nowadays, mostly about climate change, reduction of emissions related to industrial activities are of great interest. It is known that offshore activities such as oil exploration and cargo transportation can be a significant source of pollutant emissions. Thus, the research and utilization of new cleaner energy sources become very suitable. Having this in mind, this project aims to develop dynamic models of alternative energy sources to be incorporated to a dynamic model of a vessel hybrid power system integrated to the simulators of the Numerical Offshore Tank (TPN), which serves as a platform for the design and study of energy usage and emissions of a certain ship during a mission. This project focused, mainly, on developing a fuel cell model to serve as an alternative electrical energy source for a Platform Support Vessel (PSV). The models were developed using MATLAB coding environment, and basic energy conservation and mass balance equations, being designed to operate under real time conditions. Firstly, Polymeric Electrode Membrane (PEMFC) and Solid Oxide (SOFC) steady-state models were developed in order to provide a general view of the fuel cell's operational behavior and reaction mechanisms. After that, the next step was to create a transient and more sophisticated model, of not only the fuel cells, but also of a system to support fuel cell operation including a steam methane reformer and reservoir tanks. The idea was to get an overview of the fuel cell responses to transient changes such as load steps and fuel flow rate variations. In addition, after the fuel cell dynamic model is designed, it must be tested under a variety of operational configurations, with the purpose of assessing its performance and yield information about environmental performance such as ship emissions, fuel consumption and efficiency.

Poster session **# P.04**

Development of a natural gas burner using the flameless oxidation concept

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Keywords
flameless oxidation, advanced combustion, low pollutants

Impact statement
The flameless oxidation concept is one possible alternative to reduce pollutants emission from combustion systems. Although a complex physical phenomena, the operation and manufacture of the combustion chamber are simple which makes it a viable technology for easy implementation in the near future.

Highlights
Advanced combustion regime for low pollutant emission.
Labscale combustion chamber of 10kW.
Advanced laser measurements of instantaneous velocity field.
Turbulence assessment for transition and stability of combustion regimes.

Abstract
The flameless combustion regime is one possible alternative for lowering pollutant emission compared to conventional flame regime in combustion processes (Perpignan et al., 2018). To achieve the flameless regime, the reactants temperature must be greater than the mixture autoignition temperature (Wunning and Wunning, 1997) and one proposed way is by recirculating the hot combustion products to mix with the fresh reactants (Cavaliere and de Joannon, 2004). This work presents the study of main characteristics of the flow field in a flameless combustion chamber assessed by PIV. A non-reactive flow case of a laboratory scale flameless combustion chamber of 10kW was chosen for validation of the experimental test bench and measurement technique. The flameless combustion chamber manufactured was based on the design of Veríssimo et al. (2011). Detailed information about the geometry can be found also in Veríssimo et al. (2015). Solid seeding particles of Silicium dioxide SiO2 were used with a 527 nm frequency-doubled dual-cavity Nd:YLF Litron Lasers LDY302. Particle images in a Field-of-View (FOV) of 100x62 mm2 were acquired by a 12-bit CMOS camera (double-frame: 5µs) at 1.6 kHz acquisition rate for 2.38 s. The image acquisition is performed with a 527±5 nm bandpass optical filter mounted on the lenses to reduce the interference of ambient light. Laser and camera are synchronized with the pulse delay generator model 575-8C (Berkeley Nucleonics Corporation) and controlled by Dynamic Studio software (Dantec Dynamics A/S) in the acquisition computer. Planar two component (2D2C) velocity field was estimated by the adaptive cross-correlation algorithm resulting a spatial resolution of 0.6 mm. Averaged velocity components and estimated Reynolds stress tensor components obtained using PIV are compared with a CFD simulation. Important characteristics of the flow field in the flameless combustion chamber as the recirculation zone, velocity magnitudes and Reynolds Stress tensor components were observed.

Poster session **# P.05**

Numerical analysis of differential diffusion effects and determination of flammability limits in methane oxy-fuel combustion using detailed chemistry

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Keywords
Flammability limits for oxyfuel flames; Differential diffusion in oxyfuel flames; Numerical simulation of oxyfuel flames

Impact statement
Is it shown that the flamability limits for CO2 diluted oxyfuel flames are significantly narrower than for conventional flames

Highlights
This is the first time that the numerical simulations are based on free propagating flames

Abstract
The substitution of air to mixtures rich in oxygen significantly simplifies the capture of carbon dioxide in flue gas of combustion processes. The absence (or small amounts) of nitrogen in combustion products reduces the separation efforts associated to the high dilution of CO2 in air-blown processes. Nevertheless, the modification of the oxidizer composition imposes new challenges to the design and control of combustion chambers. The present work focuses on the investigation of differential diffusion effects in oxyfuel methane flames using various oxidizer compositions. Analyses are conducted using the Computational Fluid Dynamics (CFD) and a detailed description of the chemistry. Different from the previous listed works, analysis are performed considering freely-propagating flame reactors. Special attention is given to the determination of flammability limits and flame propagation speeds for cases where the differential diffusion is considered, as well as in cases where the unity Lewis simplification is assumed. Analyses are also conducted for air-blown operating conditions in order to set reference cases for the investigated scenarios.

Poster session **# P.06**

Methane tri-reforming: gas hourly space velocity and feed composition studies over Ni/CeZrO2/MgAl2O4 catalyst

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Keywords
CO2 Utilization; Syngas; Hydrogen Production

Impact statement
The study reports the Methane Tri-Reforming (MTR) versatility to generate H2+CO mixtures (syngas) with a wide range of H2/CO compositions. It was possible to adjust the syngas composition into the desired value by tuning the feed reactor composition (CH4:CO2:H2O:O2 ratios), as well as improving CO2 conversions, which is of high importance for CCSU (CO2 Capture, Storage and Utilization) policies.

Highlights
Among the ratios O2/CO2 evaluated, the value of 0.17 could be considered proper, once the CO2 conversion was kept at around 60%, while H2/CO = 1.75.
The decrease of the ratios H2O/CO2 from 1.4 to 0 led to the increment of the CO2 conversions.
Changing the O2/CO2 and H2O/CO2 ratios in the feed stream modified the composition of the produced syngas, assuming wide applications.

Abstract
The catalyst used for the studies was a nickel supported on MgAl2O4 spinel, promoted with CeZrO2 (nominal Ce/Zr molar ratio =4). Nickel content was 9.2 ±0.4 %wt and Ce and Zr loads were 13±1.0 and 2.4±0.2 %wt, respectively. Gas hourly space velocity (GHSV) tests were made by keeping the reactants flow at the ratio 3 CH4: 1 CO2: 1.4 H2O: 0.5 O2:2 N2 (CH4= 0.0021 mol.min-1), and changing the mass of the catalyst charged into the reactor. Each GHSV test was run for 5 h at 750oC and atmospheric pressure. The mass of catalyst used was: 43, 85, 113 and 150 mg, corresponding to the following GHSV's: 7.74, 3.92, 2.95 and 2.22 molreactants.gcat 1.h 1, respectively. The contact time between the reactants molecules and the catalyst is shortened with the increment of the GHSV. Hence, reactants conversions decreased, once the adsorption and molecules activation occurred less expressively. Besides, no expressive CH4 and CO2 conversions changes were observed by modifying the GHSV from 2.95 mol.gcat 1.h 1 to 2.22 mol.gcat 1.h 1(CH4 conversion ~77% and CO2, 52%). Thus, GHSV = 2.95 mol.gcat 1.h 1 was kept to study the effects of the O2/CO2 and H2O/CO2 in the feed stream. Reaction tests varying the molar ratios O2/CO2 and H2O/CO2 in the feed were made by keeping the same GHSV (2.95 mol.gcat 1.h 1. The effects of changing the ratios O2/CO2 were evaluated using the correspondent values: 0, 0.17, 0.5 and 1.5. The tests varying the ratios H2O/CO2 were made similarly, using the proportions H2O/CO2 as follows: 0, 0.84 and 1.4. Each test was also run for 5 h at 750oC and atmospheric pressure. Despite increasing O2/CO2 from 0 to 1.5 had diminished the coke deposition as well as incremented the H2/CO values, due to the POM occurrence, a drastic decrease of the CO2 conversions was observed. This last fact is not desirable, considering the importance of the CO2 mitigation from the atmosphere. Among the ratios O2/CO2 evaluated, the value correspondent to 0.17 could be considered proper, once the CO2 conversion was kept in a value reasonable high, at around 60%, while H2/CO = 1.75. Similar to the effects of changing O2/CO2 ratios, CH4 conversion (~70 %) almost did not change with the increment of the H2O/CO2 from 0 to 1.4, once the ratios between the gasifying reactants and CH4 were kept the same for all tests. CO2 conversions decreased from 73% to 30%, because the increment of the H2O/CO2 ratio in the stream favors the steam reforming (SRM) over the dry reforming of methane (DRM).

Poster session **# P.07**

Performance analysis of a water ejector using CFD simulations and mathematical modeling

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Keywords
Ejector, performance analysis, mathematical modeling

Impact statement
A one-dimensional (1D) mathematical model can be used as a powerful tool for preliminary analysis of ejetors before conducting experiments or CFD simulations, contributing to reduce costs and computational time. It can be useful to calculate the ejector friction loss coefficients, to delimit the ejector envelope of operation and to predict its maximum efficiency point using CFD results.

Highlights
The 1D mathematical model has shown to be a reliable tool to calculate the friction loss coefficients of each ejector component (nozzle, suction chamber, mixing section and diffuser), to predict the ejector maximum efficiency point and to delimit the ejector envelope of operation. For low entrainment ratio (M) values, the ejector efficiency curve is not significantly affected by friction losses.

Abstract
Ejectors are mechanical devices that transfer momentum from a high-pressure fluid to a low-pressure fluid without requiring external energy. Their structure is composed by a nozzle, a suction chamber, a mixing section and a diffuser. In this study, a one-dimensional (1D) mathematical modeling was employed to estimate the friction loss coefficient of each ejector component, to delimit its ideal efficiency (envelope of operation) and to predict its maximum efficiency point. Pressure and velocity data were extracted from Computational Fluid Dynamics (CFD) results and were employed for testing the accuracy of the mathematical modeling. Results show that mathematical model presents good agreement with CFD results and could accurately delimit the envelop of operation and predict the ejector maximum efficiency point.

Poster session **# P.08**

Tri-reforming of methane over Ni supported on CeO2 synthetized using ionic liquid: H2 selectivity enhanced and sintering resistance

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Keywords
Syngas, tri-reforming, Ni-CeO2

Impact statement
Natural gas is used in a variety of chemical process, such as energy production by combustion, syngas feedstock for long chain chemicals production and is considered an alternative for fuels derived from carbonaceous raw material. New technologies for natural gas conversion are growing considering that greenhouse gases needs to be extinguished.

Highlights
CeO2 support have an improve in the porosity by ionic liquid in the synthesis medium
Ionic liquid concentration has influence in the CeO2 basicity
CeO2 synthesis conditions affect the metal-support interaction
Ni-CeO2 catalysts with high oxygen vacancies concentration has high H2 selectivity
Ni-CeO2 synthesis conditions has influence in the metal stability

Abstract
The mitigation of CO2 and the natural gas conversion simultaneously is possible by the tri-reforming reaction in which syngas with molar ratio of 2:1 could be obtained directly. The tri-reforming reaction is an alternative to convert the greenhouse gases as a feedstock. Ni are the most used and the cheapest catalysts that are active for methane reforming reaction. Nevertheless, Ni catalysts are easily deactivated by sintering and carbon deposition. To improve Ni catalysts, different support are used and ceria is one of rare earth most used in many catalytic reactions. Because of special properties of ceria such as stable fluorite structure and different oxidation states, Ni-CeO2 may be proposed as a promising alternative. The potential to modify the size, shape and porosity of CeO2 by ionic liquid (IL) makes them interesting as a support, considering that physicochemical properties improves metal-support interaction, oxygen vacancies formation and consequently the catalytic performance. Thus, the purpose of this work is to study the influence of physicochemical properties of Ni-CeO2 catalysts. The catalysts were prepared by the ionothemal technique, varying the ionic liquid concentration. XRD, N2-physisorption, TPR, XPS and XANES techniques have been used to characterize the catalysts in order to identify the effect of selected preparation variables on morphological and structural properties of the obtained materials. The catalytic activity in tri-reforming of methane were conducted at 800 °C, with the reagent feed molar ratios of CH4: CO2: H2O:O2 at 1.0: 0.33: 0.33:0.16. The results show that part of the Ni is reduced and remain in metallic state during the reaction tests according to the support synthesis conditions. On the other hand, Ni2+ species in strong interaction with Ce cations are observed even after exposure to methane. Both Ni species and oxygen supply by the solid play important roles on reactants conversion and H2 and CO yields. Ni-CeO2 interaction is a crucial parameter for prevent sintering.

Poster session **# P.09**

EFFECT OF CH4/CO2 RATIO IN THE METHANE TRIREFORMING OVER METALLIC CARBON NANOTUBES CATALYSTS

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Keywords
Carbon nanotubes; methane;trireforming

Impact statement
Synthesis of catalysts from nanoparticles (inside and outside) carbon nanotubes.
Understand the limitations and advantages of the methane trireforming reaction.
Verify how reagent (CO2) interpose with the reaction using carbon nanotube structures.

Highlights
Synthesis catalysts Nanoparticles Carbon Nanotubes Methane trireforming reaction

Abstract
Carbon dioxide is a gaseous compound, which is also considered to be one of the main greenhouse effects causes. To facilitate decreasing and/or avoiding high CO2 emissions related to energy production and use, particular attention is paid to CCU processes, where CO2 can be used as feedstock in syntheses of desirable chemicals. One process that may utilize CO2 is the methane tri-reforming (TRM), delivering synthesis gas (H2/CO) in the presence of suitable catalyst. Thermodynamic trireforming calculations showed that high CH4 and CO2 conversions are possible. Moreover, the biggest advantage of the process is the production of synthesis gas that may be converted into methanol (MeOH) and liquid fuels (via Fischer-Tropsch synthesis). The syngas obtained in methane tri-reforming process has molar ratios in the range of 1.5 –2.0. Nanostructured materials have been studied in reforming processes. Approaches to improve catalyst life during the reforming reaction include: high dispersion of active metals; high surface area of supports; high metallic surface area, and supports with high oxygen mobility. In general, the inert support presents high porosity, high thermal conductivity and mechanical strength. The initial conditions of the catalyst, as synthesized and characterized, are not necessarily relevant, and it is very important to investigate the changes observed during the reaction for long-term tests, using modern tools of in-situ characterization, which are sensitive to structural and surface modifications. Such information is very valuable for identification of new stable materials for trireforming process. Carbon filaments are known to be formed during methane trireformig (TRM). If carbon nanotubes formation is unavoidable why not using directly carbon nanotubes (MWCNT) as support for metallic sites? It is surprising that only recently those studies using carbon nanotubes in methane reforming have appeared. In this paper, we use a selective mode of metal addition in MWCNT (multiwall carbon nanotubes) functionalized as bimetallic catalyst (Ni@MWCNT/Ce) and a scenario is discussed: TRM as an effective way of chemical utilization of CO2. In this discussion we cover the behavior of the methane trireforming reaction (regarding conversion, selectivity and H2/CO ratio) against the different feed ratios (CH4/CO2) and process temperatures.

Poster session **# P.10**

Low pressure hydrogenation of CO2 to methanol over Ni-Ga alloys and a DRIFTS analysis.

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Keywords
CO2 hydrogenation; low pressure; DRIFTS

Impact statement
The increase in global demand for methanol and the continued growth expected in the next years makes necessary to develop more selective and low-cost routes for its synthesis. With this in mind, the hydrogenation of CO2 to methanol may be a more sustainable route, consuming CO2 and obtaining a product for which there is an ever-increasing demand and that is currently derived from a fossil source.

Highlights
The presence of surfactant improved methanol productivity.
Ni-Ga alloys presented activity at ambient pressure.
Smaller particle size led to higher methanol selectivity.
Higher Ni5Ga3 crystalline phase led to higher methanol selectivity.
The mechanism on Ni-Ga alloys proceeded by formate and RWGS routes.

Abstract
Ni-Ga alloy catalysts were synthesized by a surfactant-assisted co-precipitation method and were tested in CO2 hydrogenation to methanol at 10 bar and at ambient pressure. The presence of surfactant in the synthesis led to a decrease in particle size, with the catalyst produced using 1% of surfactant (C_1%) presenting the smallest and most homogeneous particle size. A difference between the catalysts was also observed in the change of the crystalline phase after the reaction, where the C_1% catalyst presented the lowest loss of the Ni5Ga3 active phase. Methanol productivity showed positive relations with smaller particle size and higher quantity of Ni5Ga3 crystalline phase remaining after the reaction, with the C_1% catalyst presenting the highest methanol productivity. Catalytic evaluation under different conditions showed that higher temperatures and GHSV values led to poorer selectivity to methanol. The C_1% catalyst also presented good activity at ambient pressure and remained stable after 5 h, with no deactivation. A mechanistic study employing DRIFTS analyses found that the reaction pathway on Ni-Ga alloy involved both the RWGS and formate routes, as shown by the presence of formate, methoxy, and CO intermediates.

Poster session **# P.11**

Development of heterogeneous single-metal site catalysts for partial oxidation of methane

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Keywords
methane; methanol; single-metal sites.

Impact statement
The abundance and environmental concerns related to emission of methane into the atmosphere have intensified research for valorization of this gas in recent years. Currently, processes that efficiently convert methane to alcohols are complex and costly, since they envolve indirect routes and high temperatures. In this scenario, direct conversion emerges as a promising alternative.

Highlights
Low temperature activation of methane and conversion to methanol over Rh/CeZrO2 catalysts; Rhodium single-site stabilizes CH3 intermediates after methane activation; Ordered mesoporous ceria-zirconia supports present high surface area to better disperse rhodium.

Abstract
One of the major products in the direct transformation of methane is methanol, one of the most important raw materials in the global industry, which has shown increasing annual demand. Motivated by the current scenario of high availability and immediate search for valorization processes, this work presents the development of single-atom noble metal catalysts supported on mesoporous cerium-zirconium dioxides for direct and efficient conversion of methane to methanol under mild reaction conditions. Unlike nanoparticles, that tends to completely dehydrogenate methane molecule, atomically dispersed noble metal sites can stabilize CH3 intermediates after first dehydrogenation of methane, favoring the formation of methanol under the presence of an oxidant compound. In the present contribution, catalysts comprising Rh sites over CeZr supports were evaluated on partial oxidation of methane to methanol. Preparation of ordered mesoporous ceria-zirconia supports were based on a sol-gel process combined with evaporation-induced self-assembly (EISA) in ethanol using Pluronic P123 amphiphilic triblock copolymer as the structure-directing agent. Rhodium was atomically dispersed over supports by impregnation applying strong electrostatic adsorption (SEA) method. Structural and textural properties of catalysts were evaluated by X-ray diffraction and nitrogen physisorption isotherms to confirm the presence of hexagonal mesopores and crystalline walls containing the mixed oxide phase. Nature of rhodium sites deposited over supports was evaluated by in situ Fourier transform infrared spectroscopy using CO as a probe molecule, since this compound adsorbs on different ways over isolated sites or nanoparticles. Catalytic tests were carried on a batch reactor under 30 bar of CH4 and using H2O2 as oxidant at 70°C. The low activation energies and capacity to stabilize methanol intermediates provided by the single-atom sites associated with high oxygen storage capacity and mobility, characteristic of ceria-zirconia supports, were determinant properties to obtain efficient catalysts for the process.

Poster session **# P.12**

Production of Olefins by Fischer-Tropsch Synthesis using Structured Reactors

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Keywords
Fischer-Tropsch Synthesis, Structured Reactor, Olefins

Impact statement
The study focuses on the improvement of the Fischer-Tropsch Synthesis (FTS). While most studies in the literature focuses on improving FTS by developing novel catalysts with better conversion and selectivity to the desired products, our focus isover the reactor technology.

Highlights
The SBA-15 suspension for monolith coating was prepared and characterized; The 15%Co/SBA-15 catalyst performance for the Fischer-Tropsch Synthesis reaction was evaluated through a catalytic test.

Abstract
Energy is one of the most important resources for mankind's development. We are facing a shift of primary energy sources towards renewables due to the negative environmental impacts of our current energy matrix. Natural Gas (NG) stands out in this transition scenario, since it is a cleaner fossil fuel. In this context, the gas-to-liquids (GTL) technology plays a strategic role, since a wide variety of hydrocarbons, such as paraffin, olefins and oxygenates, can be produced from NG. Fischer-Tropsch Synthesis (FTS) is the core process of GTL. It is a complex, triphasic and exothermic reaction, which requires improvements in different scales in order to improve the reaction performance. The literature shows that the use of structured reactors leads to the increase of heat and mass transfer in the system. Moreover, the use of honeycomb monolith as a primary support significantly improved the overall reaction performance, although most studies were performed using a standard catalyst for this reaction, which is the (un-)promoted Co/Al2O3. In this context, this study proposes the development of cordierite monolith reactors using an advanced cobalt-based catalyst over SBA-15 as secondary support for the FTS reaction, for the production of light olefins. The SBA-15 support and 15 wt.% Co/SBA-15 powder catalyst have been synthesizedand characterized. SBA-15 suspension features for cordierite monolith anchoring have also been evaluated. Techniquessuch as Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), N2-sorption Isotherms, X-Ray Diffraction analysis (XRD), Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES), Hydrogen Temperature Programmed Reduction (H2-TPR) and Stabilization Analysis were applied. The 15% Co/SBA-15 catalyst performance was also evaluated using an automated fixed bed reactor (Microactivity Effi, PID Eng. Tech), coupled to a Gas Chromatograph (Shimadzu) at 250 °C and 21 bar. Results from the preparation of the structured reactor shows that the used approach did not result in a relevant adherence of the secondary support, hence the increase of surface area of the cordierite monolith prior to coating may improve efficiency. The catalytic test shows that the catalyst produces mainly paraffins on tested operational conditions. The addition of promotors, the modification of the catalyst's and cordierite monolith's surfaces and the modification of space velocity may lead to a shift to light olefins selectivity.

Poster session **# P.13**

DRIFTS Study on Lanthanum Promotion of a Co-based Supported Graphene Catalyst

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Keywords
Graphene, Fischer-Tropsch Synthesis, DRIFTS

Impact statement
Graphene is one of the most studied carbon nanomaterials due to its remarkable properties. While several works using graphene as support for catalytic applications have been done, Fischer-Tropsch studies using this carbon allotrope are scarce and even inconclusive. So, this study is focused in evaluate graphene catalytic performance and lanthanum promotion role on Fischer-Tropsch Synthesis mechani

Highlights
High quality graphene sheets were synthesized. Cobalt nanoparticles were deposited over graphene surface . Cobalt nanoparticle average size of 13 nm was obtained, which is suitable for FTS application. Lanthanum promoter was successful incorporated on catalyst. Fischer-Tropsch Synthesis mechanism over the designed catalysts was evaluated by DRIFTS and Mass Spectroscopy.

Abstract
Fischer-Tropsch synthesis is the catalytic conversion of synthesis gas to high quality hydrocarbon fuels. The catalyst design plays an important role in FTS operation costs. Aspects such as the catalyst activity and selectivity for desired products should be further investigated for process feasibility. Since early works, it is known that Group VIII metals are very active in CO hydrogenation, mainly Co and Fe. Co-based catalysts are preferred, since they are more active than Fe-based ones and require lower reaction temperature. Some inorganic supports with high surface area such as silica, alumina and niobium oxide have been used to increase cobalt dispersion. FT industrial plants use cobalt on alumina catalysts for long-chained alkanes production even at mild conditions. However, the formation of irreversible cobalt-aluminates during pretreatment and under reaction conditions leads to the catalyst deactivation. In this context, carbon nanomaterials have gained prominence due to their notable properties, such as high mechanical resistance, high superficial area, thermal stability and high electronic conductibility, making these materials promising supports for heterogeneous catalysts. Recent studies also indicate that metal nanoparticles supported on carbon nanomaterials used in FTS showed high activities for C5+, as well as low selectivity for the formation of methane and CO2 and avoid cobalt mixed-oxides formation. High surface graphene as a support for cobalt promotes a better nanoparticles dispersion and its surface defects may be sites for adsorption of active species for catalysis process. Promoting effects due to the presence of a second metal over reducibility, activity and stability of cobalt catalyst have been reported in numerous studies. Rare earth promoters such as La, Ce, Pr and Sm are also investigated, since they may improve Co-based catalysts performance, decreasing methane production and increasing the selectivity for C5+ and catalyst stability. Therefore this work is focused in designing a cobalt-based catalyst promoted with lanthanum and supported on graphene for Fischer-Tropsch Synthesis. The materials were characterized by different techniques such as surface area measurement, XRD, Raman spectroscopy, HRTEM for structure and properties verification. Reactants adsorption and products formation mechanisms were evaluated by Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) technique and online Mass Spectroscopy.

Poster session **# P.14**

General principles of Law: applicability in CCS activities

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Keywords
Law Principles. Carbon Capture and Storage. Environmental and Economic Law.

Impact statement
The general principles of law are basic and general directives guiding the interpreter applying the right in case of omission of the legal text. The principles establish values and constitutional assets that begin to be the basis of legal norms and the work proposes reflection on which of them are related to CCS activities.

Highlights
'- The general principles of law are basic and general directives guiding the interpreter applying the right in case of omission of the legal text. - Many principles in the right of the International agreements. -The Kyoto protocol and the Paris Agreement shall be an increasingly clear sense of development based on environmental protection and the reversal of the effects of greenhouse gas emissio

Abstract
The present work proposes a reflection on principles applicable to Carbon Capture and Storage (CCS), within the perspective of Constitutionalization of Law and considering the intersection between Environmental Law and Economic Law and the hermeneutic process of integration of legal norms. The method used was the deductive, starting from the general principles of the law for the principles of law related to the activities of Carbon Capture and Storage, through interpretative technique and bibliographic and documentary analysis.

Poster session **# P.15**

Digital CCS Plants in a e-Sustainable world

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Keywords
CCS, Digital Transformation, Energy Transition

Impact statement
Disruptive Digital Transformation for a smart Energy Transition

Highlights
eSustainability - Balancing the Energy Trilemma with Digital Innovation
Digital CCS Plant: challenges and opportunities

Abstract
This works brings a Digital CCS Plant proposal to exhibit the benefits of embracing Digital Transformation on Energy Transitions and how its implementation can help us reach our common net-zero carbon emissions goal without losing industry and society value. Furthermore, acknowledging that Digital Transformation must present through all the value chain, this work analyses the role of digital innovation in new energy sources and its benefits regarding operation, finance and risk.

Poster session **# P.16**

Comparative International Law: the scope and management of public participation rights related to CCS activities

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Keywords
Comparative International Law; Public Participation; Carbon Capture, Transport and Storage.

Impact statement
It is important to understand of whether and how specific jurisdictions deal with particular issues associated with CO2 storage. The paper proposes the presentation of the item of public participation in the regulatory standards of CCS existing in Australia, Canada, the European Union, the United Kingdom and the United States and their possible relations with the Brazilian configuration.

Highlights
Participatory democracy is based on international treaties received by the Brazilian legal system.
The standards studied mention the right to publicity of records, licenses and activities related to CCS activities as essential.
CCS legislation to be implemented in the country could adopt process of participation, conferring powers of intervention and deliberation.

Abstract
The paper proposes the presentation of the item “public participation” in the CCS regulatory rules existing in Australia, Canada, the European Union, the United Kingdom and the United States, consolidated jurisdictions on the subject, and their possible relations with the Brazilian configuration. The choice of jurisdictions is due to the existence of the item in its legal and /or regulatory rules. Thus, it makes use of the law compared to normative and bibliographic research and proposes that the item public participation be considered in future CCS standards that may apply in Brazil.

Poster session **# P.17**

Synthesis and characterization of composite ceramic membranes (zeolite /alumina) for separation of carbon and methane gas

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Keywords
CO2/CH4 separation; Zeolite / alumina membranes; Co-extrusion

Impact statement
The development of double layer hollow fiber membranes is a way to reduce the use of expensive materials. The problem faced today is the complexity involved in the production of the support layer and then a complementary treatment of it, which makes production process more expensive. Thus, the use of simultaneous co-extrusion can reduce the cost of producing double layer ceramic membranes.

Highlights
Purification of natural gas is necessary for expanding its use by the industry and other commercial activities Double layer membranes have advantages over single layer membranes Ceramic membranes are advantageous over polymeric membranes Simultaneous extrusion is still a problem due to the numerous process variables

Abstract
The exploration of the pre-salt in the Brazilian coast will increase the production of oil and natural gas. Natural gas is composed mainly of methane gas (CH4) and carbon dioxide (CO2), the CO2 reducing the calorific value of the mixture, limiting its application in industrial activities and combustion processes. The use of membranes for separation of gases is a technology that has aroused industrial and scientific interest due to its efficiency and lower energy consumption compared to other technologies currently employed. The aim of this work is the development of composite membranes, zeolite/alumina, by co-extrusion, in the configuration of hollow fibers for the separation of CO2 and CH4. The manufacture involves the production of zeolite and alumina (Al2O3) suspensions in polymer solutions (Polyethersulfone (PES)/N-methyl-2-pyrrolidone (NMP)/Additive) for casting hollow fiber membrane by simultaneous double extrusion, phase inversion by immersion and calcination. Single layer alumina membranes were fabricated in order to verify the best solution composition (PES, NMP and additive percentage) and the mechanical resistance of the membrane. The maximum concentration of polymer, in which the viscosity was altered, was 1% by weight. It was verified the necessity to acquire alumina with smaller size particle (<1 µm) for sintering. With the new alumina it will be possible to prepare and to characterize dope solutions and cast membranes. Dope solutions and prepared membranes will be characterized through viscosity evaluation, membranes internal and surface structures, surface area and porosity, mechanical strength, and separation capacity. Zeolite/alumina membranes are expected to be stable and durable in the long term, and thus can be employed on an industrial scale.

Poster session **# P.18**

Solving the wave equation with exponential integrators

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Keywords
wave equation, exponential integrator, direct problem

Impact statement
The application of an exponential integrator method to solve the wave equation is a promising area in seismic exploration because of its high accuracy properties and easy parallelization in time.

Highlights
Formulation of the PML absorbing boundary condition to the wave equationTransformation of material parameters to reduce numerical error in heterogeneous materialsNumerical experiments verifying PML condition and the parameter transformation in a heterogeneous mediumExponential Integrator for the wave equationComparison of the exponential integrator method with the solution an explicit method

Abstract
In this study, we discuss numerical methods to solve the wave propagation equations in a heterogeneous medium, a popular approach in the area of seismic mapping. But to approximate the solutions of the wave equations embedded in a heterogeneous medium and simulate an infinite space, numerical considerations are required. An Absorbing boundary condition to mimic an infinite domain while working with a finite one, and a transformation of material parameters near discontinuities, to improve the quality of the approximation, were developed. Next, an explicit numerical method based on finite differences is used within examples to verify the expected theoretical results and to study the solutions of the wave equation. Furthermore, a new approach to calculate solutions of the wave equation, based on exponential integrators, is presented, discussing its advantages and principal challenges.

Poster session **# Q.01**

Changes and Innovations in the Regulatory Framework of Natural Gas: overview and review of current literature on the subject.

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Keywords
Natural Gas; Regulatory Framework; Gas Law

Impact statement
The necessity to keep up to date and review the literature that has been published, lies in the importance of being aligned with the trends of the natural gas sector. Furthermore, in order to expand its use as a Brazilian energy matrix, it is essential to know the regulatory aspects that, if better adjusted and implemented, will be able to liberalize and expand the limits of the gas market.

Highlights
This is a review of selected articles from the book "The Natural Gas Regulation in Brazil", released in 2019, which focus on the most recent discussions that permeate the regulation of natural gas and the innovations implemented in it, as well as the practices capable of improve exploration and knowledge of this sector.

Abstract
Natural gas has been placed as the fuel of the energy transition because it presents a high energy efficiency while emitting less greenhouse gases when compared to other fossil fuels. This characteristic is a differential for encouraging the use of natural gas as a substitute for other fossil fuels, both in the transport sector and for the generation of electricity and heat. Brazil, after the discovery of the pre-salt reservoirs, became an petroleum exporting country and a potential major natural gas producer, since these reservoirs are associated with gas. However, the regulatory framework, the infrastructure for gas commercialization and the increasing demand for this energy source in the country are in the maturation phase. This article reviews the latest movements in the sector and actions to enable the expansion of the use of natural gas in the Brazilian energy matrix that have been addressed in scientific articles written by experts in the field. This article congregates the main changes in the gas regulatory framework, from the Gas Law (Law No. 11.909/2009) to the most recent movement, Resolution 16 of the CNPE, which established the New Gas Market, and shows that the revised literature has pointed to regulatory innovations and the existence of uncertainties and points of conflict in legislation at all levels of the gas chain: production, transportation, distribution and commercialization.

Poster session **# Q.02**

RCGI Lex as a tool to disseminate knowledge about gas legislation and contribute with the Sustainable Development Goals

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Keywords
Energy Law, Sustainable Development Goals (SDG), Gas Legislation

Impact statement
RCGILex provides information service by organizing the Brazilian and Paulista Natural Gas law in a comprehensive perspective. It is a digital Law Centre with an extensive compilation of the federal and state level regulations commented by experts. RCGILex is an open-source tool available to everyone interested in the gas sector legislation and contributes towards the SDG of the Agenda 2030.

Highlights
'-RCGILex is a digital Law Centre assessable to everyone. -Brazilian and Paulista Natural Gas service disseminates knowledge. -Natural gas is seen as a transitional fuel to cleaner and sustainable energy. -RCGILex is building paths towards the SDGs of the Agenda 2030 of the United Nations. -Education, equality, justice, innovation, partnership are some goals pursued by RCGILex project group.

Abstract
The aim of this work is to present the efforts of the RCGI's project 21 – creation of Brazilian and São Paulo legal service - to contribute towards the implementation of the Sustainable Development Goals of the United Nations. Through the creation of a collaborative digital Law Centre, that enables availability of gas legislation to experts, law students and laypeople, it disseminates knowledge about natural gas as a sustainable transitional fuel towards a cleaner energy mix. The aggregated approach of the RCGILex website and the RCGILex tool nurtures discussions about Brazilian and São Paulo legislation in the gas sector and promotes seminars, supported by newsletters, reports and white papers as well as a journal. By means of an analytical framework methodology evidences are presented of related results that impact on the goals of the Agenda 2030 in Brazil mainly in quality education, gender equality and inclusion, industrial innovation and infrastructure, partnerships, peace and justice, cleaner and affordable energy and climate change mitigation.

Poster session **# Q.03**

SÃO PAULO STATE ENERGY SECTOR CO2 EMISSIONS: SIMULATION MODEL CONSIDERING THE 2040 MACROMETROPOLE PAULISTA ACTION PLAN

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Keywords
LEAP MODEL, GHG EMISSIONS, SAO PAULO STATE

Impact statement
This paper novelty regards on the simulation of the Macrometropole Paulista Action Plan (PAM, 2014) structural interventions projects for the São Paulo state energy sector from 2014 until 2035 ans its potential impacts in the GHG São Paulo emissions

Highlights
Model's results presented possible benefits of 8% less GHG emissions compared to the São Paulo state baseline scenario; Local electricity generation increase around 18%.

Abstract
Meeting countries National Determined Contribution (Paris Agreement, 2015) will require not only the development and application of advanced low carbon energy technologies, but also a robust effort to rethink new structures and new energy planning process. In this sense, urban regions are strategic place to implement climate change mitigation and adaptation strategies through local and/or regional energy planning aimed at reducing CO2 emissions and energy demand. This paper presents a simulation model for the São Paulo state transformation sector by applying the Macrometropole Paulista Action Plan (PAM, 2014) structural interventions projects focused on increasing the electricity generation installed capacity from 2014 until 2035 and its impact in terms of GHG emissions. The PAM structural projects implementation increases the thermal powerplants installed capacity in 88% - 18,551MW (for powerplants using natural gas and biomass), and according to the model's result, the implementation of such projects will incur in a 3% local emissions increase compared to the current scenario (Baseline). On the other hand, the São Paulo state global emissions will be reduced by around 8%, considering the electricity imports reduction (associated with an average grid emission factor of 0.10 tCO2, kept constant) due to the increase in local electricity production when compared to the Baseline scenario.

Poster session **# Q.04**

Estimating thermoelectric dispatch for the Brazilian Electricity Sector 2019-2030 from the 2027 Ten Year Expansion Plan: a stochastic dual dynamic programming (SDDP) approach

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Keywords
Natural Gas, Thermoelectric Dispatch, Energy Balance

Impact statement
Environmental and technical thresholds of renewable energy sources expansion in the Brazilian Electric System tend to increase thermoelectric dispatch by four (4) times, compared to 2019, an optimistic rainfall scenario. Hence, there is a promising potential market for Carbon Capture and Storage and carbon pricing in Brazil in the next decade.

Highlights
The increasing share of renewable sources in the Brazilian electrical matrix tends to increase thermoelectric dispatch, especially, of those run NG. Using the inputs of PDE 2027 and four rainfall scenarios for the period 2019-2030, this paper estimates an increase of between 200% and 400% of NG dispatch, depending on the scenario. Hence, there is a promising potential market for CCS.

Abstract
The Brazilian Electricity Sector (BES) is organized as a hydrothermal system with a predominance of hydraulic generation (66%). Thermoelectric generation participates as a complementary source in the National Interconnected System (SIN) and accounts for 25% of the supply. Due to the persistent drought of recent years, however, thermoelectric plants are being dispatched more frequently than initially planned, generating additional costs for society. In addition, it is expected that recurrent thermoelectric dispatch will become increasingly frequent in the future due to: (i) environmental issues given that Brazil is near the limit of the expansion of hydropower plants with reservoirs; and (ii) the increasing share of intermittent renewable sources in the matrix, including watercourses, solar and wind. In this context, the objective of this paper is to estimate the thermoelectric dispatch for the Brazilian Electricity Sector 2019-2030 from the 2027 Ten Year Expansion Plan using a stochastic dual dynamic programming (SDDP) approach, called NEWAVE, and three additional scenarios considering the average rainfall of the last five (5), 10 and 15 years. The results indicate an expressive increase of thermoelectric dispatch, especially of the natural gas power plants, followed by coal, and fuel oil. In the stochastic scenario, the NG dispatch increases more than 200% vis-a-vis a 54% increase of the electricity load. In the other scenarios the NG dispatch grows more than eight (8) times. Therefore, the thresholds of renewable sources expansion in the BES significantly expand thermoelectric dispatch compared to 2019 and indicate a promising potential market for carbon capture and storage (CCS) and carbon trading systems in the next decade.

Poster session **# Q.05**

The implementations of public policies and the use alternative fuels to a low-carbon transition in Brazil

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Keywords
Public Policies; Alternative Fuels; Low-Carbon Transition

Impact statement
Identify how the Brazilian government conducted public policies actions over the last four decades in the transport sector and how the inclusion of alternative fuels has influenced in the implementation of other public policies.

Highlights
'- Identification of economic impact in the implementation of public policies in transport sector (alternatives fuels) in Brazil. - Analysis of decision-influencing agents (Brazilian federal government and its policy changes) in the implementation of public policies related to the use of alternative fuels. - The urgency of the use of alternative fuels to a low-carbon transition.

Abstract
The monopoly of gasoline and diesel in transport has caused several social and environmental impacts mainly in development countries such as Brazil. Problems as the emissions from the transport sector, which has contributed to increase the concern about the importance of diversify the energy matrix. In 1997, the transport sector was one of the highlights of the Kyoto Protocol establishing greenhouse gas emission reduction and additional mechanisms for implementing these targets. Before that, there were no specific greenhouse gas emissions reduction targets foreseen for this sector. Base on the context, climate change and reduction of CO2 emissions have been requiring a low-carbon transition mainly through the use of alternatives fuels. Over the last decade, several public policies and programs focus on the transport sector have been implemented in Brazil, which contributed to changes in the way fuels are consumed. The aim of this work is to analyze the effects of the Brazilian public policies on consumption of three alternative fuels, ethanol, biodiesel and natural gas and to perform a qualitative analysis of recent public policies for the transport sector in a contemporary context of two new alternative fuels to a low-carbon transition: biomethane and electricity. From crossing historical fuel consumption data with the implemented policies from 1970 to 2018, it was possible to identify the key policies that supported the increase of alternative fuel and which have not achieved the desired outcomes.

Poster session **# Q.06**

OPTIMIZATION OF ECONOMIC COST MODEL FOR SMALL SCALE LNG AND ELABORATION OF USER MANUAL

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Keywords
Small Scale Liquefied Natural Gas; Cost; Manual

Impact statement
The supply of gas to regions distant from the existing pipeline network requires the analysis of non-conventional logistic alternatives, such as small-scale LNG production and road transport. The cost assessment of these alternatives is essential to justify investment and assess potential profit. The model proposed by Fraga (2018) has been optimized and estimates the cost for small-scale productio

Highlights
'- Serving consumers in remote off-grid areas in Brazil - Small Scale LNG Logistics - Small Scale LNG cost model optimization - Cost model users guide

Abstract
The large reserves found in the Brazilian pre-salt and the discovery of the Argentine shale gas further increased the pool of natural gas offerers in Latin America, throwing the price of the NG down. However, for the remote regions of the pipeline infrastructure in the country, the diffusion of natural gas is extremely low. With the respective opening of the natural gas market in Brazil and the consequent increase in competitiveness, the creation of new markets for NG and the possibility of new projects in the gas sector grow. One of these alternatives is the production of liquefied natural gas in small-scale plants, which allows the service to markets in remote off-grid areas. In order to evaluate the costs for the logistic alternative of the Small-Scale LNG, the cost estimation model proposed by Fraga (2018) was optimized and a user manual was developed facilitating it's use and dissemination. The model has a total of nine tabs, of which three are for data entry (input/input) and eight for calculation and presentation of results (output). The modeling consists of the analysis of the following phases of the LNG chain, liquefaction, logistics, regasification and storage. For each of the steps the CAPEX and OPEX values are calculated from the input data provided by the user. Relating these inputs to some economic and logistical assumptions, the total cost of LNG transport is reached, in dollars per energy unit (USD/MMBTU). The result is obtained by dividing the costs of CAPEX and OPEX by the amount of LNG to be transported in energy units (MMBTU).

Poster session **# Q.07**

Social effects of a probable growth of household gas use

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Keywords
social effects; gas; growth

Impact statement
This research aims to verify how a probable growth of gas use in households can imoact social life, considering four variables: energy vulnerability, emissions, costs and technical viability.

Highlights
The growth of gas use will lead to some social impacts. What will be the effect on energy vulnerability? What will be the effect on emissions? What will be the impact on household´s energy bill? Are there some technical obstacle to the growth of gas use in households? This work aims to answer these questions, supported by mapping techniques.

Abstract
Considering the perspective of a growing use of gas in households due to the increasing production and drop of prices of this source of energy, this project aimed to forecast its effects on São Paulo dwellers. To do so, we chose four variables to analyse and to map relying on São Paulo data base and demographic census: energy vulnerability (likelihood of energy outages), sustainability (emissions), costs (energy bill) and technical viability (gas grid and availability of gas-powered devices). We analysed each variable by crossing some relevant data (indicators), calculating their values and/or using the AHP matrix. Then, we insert the results of each variable into the ArcGis software to generate illustrative maps of the probable effects of the growing use of gas. In the maps, all residential areas of the city of São Paulo was classified according to the strength of the respective effect (very high, high, medium, low). For the first variable, in the scenario of equal use of gas and electricity (50%-50%, being 73%-27% the current situation) we showed a drop of 11% of energy vulnerability. For the second variable, the map showed more emissions in densely populated areas, being 2.44% the average growth. Yet, considering the same scenario of 50%-50%, the cost of household energy bill would drop 7%. Finally, the variable technical viability showed a map with areas where the growth of gas uses would be more or less favourable. Here, we analysed only the current situation without projecting scenarios. We believe that could be used, both by the government and the gas companies to plan more efficiently the gas expansion in São Paulo.

Poster session **# Q.08**

Supercritical flow process for the Reduction of CO_2 to methanol

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Keywords
flow process, supercritical CO2, methanol

Impact statement
A supercritical flow process was developed to converto CO2 into methanol with high yield and selectivity

Highlights
IrRe/TiO2 catalyst produced methanol from CO2 in up to 32% conversion and 79% selectivity rates When tuning the reaction mix flow rate, a trade-off is made between CO2 conversion and methanol yield. Supercritical state of CO2 is important to the conversion rates. Temperature variation could avoid CO and CH4 formation

Abstract
A rather novel approach to reduce the carbon footprint is converting carbon dioxide itself directly into fuel or valuable chemicals, which can be accomplished by chemical, electrochemical, photochemical or biochemical catalysis. A myriad of products can be obtained from CO2 such as organic or inorganic carbonates, amides, urea, salicylic acid, syngas, fuel hydrocarbons or fuel alcohols. (Aresta, et al., 2013) In the present work, a continuous flow reactor system was devised and loaded with a heterogeneous catalyst, composed of iridium and rhenium supported on titanium oxide P25. A gaseous mixture of carbon dioxide and hydrogen was pressurized and pumped through the reactor, producing methanol as the major product, and ethanol as the secondary. Reaction parameters such as temperature, pressure and flow were studied and being optimized. Preliminary results show that the reaction yield was 32% whilst exhibiting 79% selectivity towards methanol when using a gas flow of 0.5 mLmin-1 of CO2:H2 mixture (1:3) at 250 °C and pressure of 100 bar.

Poster session **# Q.09**

Carboxylation of Lignin derivatives under supercritical conditions

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Keywords
Lignin, Vanillin, Carboxylation.

Impact statement
Biomass valorisation and CCSU are two different areas of research which aims sustainable energy production. This work aims to put together both areas. Lignin is a polymer from vegetable sources. One of the main components of lignin is vanillin. Larger molecules are produced by the union of vanillin CO2 from CCSU processes.

Highlights
Biomass valorisation and CCSU join together. Carboxylation of vanillin under supercritical conditions. Catalityc reaction. Different carboxylation tecniques. SCCO2 is both reactant and solvent.

Abstract
Carbon capture storage and utilization (CCSU) is considered a very relevant approach to reduce the global emissions of CO2 to the atmosphere and therefore mitigate global warming. CCSU captures CO2 from the atmosphere or the gas effluents of energy sites and either storage the CO2 in natural reservoirs or to use this CO2 as feedstock for new or current industrial processes. In parallel to the CCUS, the valorisation of biomass also reduces the production of CO2 by using biomass as feedstock instead of fossil fuels. This includes production of biofuel from vegetal sources, energy production from combustion of pellets or production of aromatic compounds from the depolymerization of lignin. This study combines biomass valorisation and CCSU: Vanillin is one of the main products on the depolymerization of lignin and therefore a relevant compound for valorisation of biomass like agricultural waste. Therefore, if vanillin (or other lignin derivative (guaiacol, cresol…) are reacted with CO2 from a CCSU process, both technologies are been used in concurrence and together might have a greater impact on abatement of greenhouse gases emissions. The objective of this study is the carboxylation of vanillin in catalytic reaction, because the obtained products might be of interest to produce new polymers from renewable sources and therefore reduce the use of oil-produced monomers. Furthermore, the carboxylation of this compound could be easily adapted to other lignin derivatives to obtain new products. The carboxylation of vanillin is produced by a catalytic reaction under supercritical CO2. Different catalysts were tested based in literature and different range of pressure and temperature to find the best possible working conditions conversion wise. Supercritical CO2 is used not only as a reactant but also as solvent since vanillin is soluble in SCCO2. In addition to this, CO2 is often used for extraction of vanillin and for lignin depolymerization. Therefore, the mixture is already under the pressure conditions required and that might save time and costs.

Poster session **# Q.10**

Tuning Nickel Catalyst selectivity in RWGS by N-doped carbon coating

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Keywords
RWGS, Nanocatalysis, Nickel

Impact statement
CO2 has a great potential as a possible cheap and abundant C1 building block for many processes in chemistry, and its conversion into CO is an important step towards hydrocarbons and olefins. Here, we have shown that undesired methane production, which is typical for high loading (big particle) Ni catalysts, could be overcome by coating the catalysts with a carbon layer.

Highlights
New strategies were studied for the application of nickel catalysts in RWGS, for CO generation over CH4. Coating with a carbon layer generated by controlled pyrolysis proved crucial for controling RWGS selectivity, leading to linear Ni-CO bonding modes. By Drift, these bonding modes are related to a shorter CO residence time on the catalyst surface, explaining their better selectivity.

Abstract
The Reverse Water-Gas Shift reaction is one of the most widely studied reactions for CO2 hydrogenation. The carbon dioxide reacting with H2 reduces to CO and also generates water. The generated CO can be used in several other reactions, such as Fischer-Tropsch for the formation of higher alkanes and olefins. RWGS is an endothermic reaction, therefore favored at high temperatures. However, when reaction occurs at temperatures below 600 ° C, the Sabatier reaction (hydrogenation of CO2 to CH4) becomes an undesirable reaction. Therefore, this work proposes to control the selectivity for CO formation in nickel (earth abundant metal) catalysts avoind CH4 formation. From previous work by our research group it was found that the coke formation on nickel catalyst surface at RWGS promote a significant improvement in CO selectivity. Thus, a complex between nickel and 1,1-phenathroline was prepared and impregnated with commercial silica in order to, after controlled pyrolysis, generate a graphical carbon layer with nitrogen-containing sites. Comparative tests were performed between the hybrid catalyst (with the organic phase) and the naked catalyst. For this, reactions were made in a fixed bed reactor, under atmospheric pressure and heating up to 800 ºC. Both showed good CO2 conversion activity, but the hybrid catalyst showed higher selectivity when using a ratio of 1 to 1 of CO2 and H2. When the ratio was increased to 1 to 4 of CO2 and H2 (more favored CH4 formation), respectively, the hybrid catalyst was even better at controlling selectivity. Then different catalysts were prepared with and without the organic phase in different supports. The best catalyst was still the hybrid supported on commercial silica and the worst catalyst on the same support, without the N-doped coating and prepared by the incipient wetness impregnation method, generating even more CH4 than CO. In order to understand the role in control in RWGS a study by Drift was performed for the best and worst catalyst. In the hybrid catalyst a large population of linear bonding modes between a Nickel atom and CO has been observed. In the naked catalyst the majority binding modes were the bi and tridentate binding modes. These two and tridentate binding modes are associated with longer residence times, so the CO is hardly desorbed as a product, remaining on the surface for subsequent hydrogenation to CH4, thus explaining its worst selectivity in RWGS.

Poster session **# Q.11**

N doped carbon embedded with Ni-Zn carbide derived from ZIF-8 for selective CO2 to CO reduction

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Keywords
CO2 reduction; Metal Organic Frameworks; Nickel and Zinc carbide

Impact statement
The use of carbon dioxide as a renewable feedstock contributes to a more sustainable use of resources and mitigation of emissions. CO2 conversion into CO is an important step towards hydrocarbons and olefins. Here, we prepared a NiZn carbide embedded in N doped carbon catalyst that suppressed the formation of undesired methane and therefore increased the yield of CO.

Highlights
Materials with high affinity with CO2 is very attractive for its reduction. ZIF-8 (a Metal Organic Framework) was exploited to prepare porous carbon materials with exceptionally high specific surface areas. ZIF-8 pyrolysis in inert conditions can produce N doped carbon material with high concentration of pyridinic N, which can capture and enrich CO2 due of its alkalinity.

Abstract
The reverse water gas shift reaction is a promising CO2 chemical conversion because of its thermodynamic favorability. CO2 is reduced by H2 generating CO which is a precursor for synthetic processes to obtain fuels, polymers and other chemicals. Herein, we prepared N-doped carbon materials by pyrolysis of ZIF-8, a framework based in imidazole coordinating zinc atoms. When ZIF-8 is calcined in inert conditions can produce N-doped carbon material with high concentration of pyridinic N, which can capture and enrich CO2 while at the same time also serve as an active site for CO2 reduction. ZIF-8 was prepared by mixing zinc acetate tetrahydrate with 2-methyl-1H-imidazole in an ammonia solution. The as-obtained sample was stirred at room temperature for 4 h before centrifugation and washing with deionized water. The sample was dried at 65 °C for 12 h. Then, ZIF-8 was calcined at 400 °C for 1 h under N2 atmosphere at a heating rate of 5 °C/min and 550 °C for 1 h at a heating rate of 2 °C/min. This sample was named ZIF-8-C. NiZn/ZIF-8-C was prepared by the impregnation method, mixing nickel(II) acetate tetrahydrate and ZIF-8 at different mass ratios. These samples were calcined under the same conditions previously described. Characterizations were performed by XPS, XRD, Raman, AA, BET, TGA, TEM, EDS and elemental analysis. CO2 adsorption isotherms were obtained at 30, 40 and 50 °C. The RWGS reaction was performed in a microreactor (CATLAB apparatus, Hiden Analyticals) equipped with a mass spectrometer. The gas composition was 2 mL min-1 of CO2, 8 mL min-1 of H2 and 90 mL min-1 of Ar. XRD and Elemental analysis showed that the pyrolysis process in inert conditions avoids oxidation of ZIF-8 to ZnO. The N1s XPS spectra of ZIF-8-C can be deconvoluted into four peaks at 398.5, 399.0, 400.9 and 403.4 eV assigned to pyridinic, pyrrolic, graphitic and oxidized N, respectively. The high content of pyridinic N leads to the higher alkalinity sites which contributes to the CO2 adsorption process. After impregnation of nickel(II) and pyrolysis, a NiZn carbide is formed (Ni3ZnC0.7). The specific surface area for ZIF-8 was 823 m2g-1, which is larger than the calcined samples. the NiZn/ZIF-8-C catalysts were very selective for CO and the competitive methanation reaction was suppressed in the whole temperature range studied. The catalysts with 5wt% Ni reached higher conversion, but the turnover frequencies of CO formation dramatically decrease with the increasing of Ni loadings.

Poster session **# Q.12**

Fischer Tropsch synthesis using hybrid iron catalysts

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Keywords
Fischer Tropsch synthesis, iron catalysts, hybrid catalysts

Impact statement
The mitigation of CO2 became subject of many studies, due to its importance in global warming. However, it is a stable molecule and it makes chemically inactive, and their activation is a vital progress to CO2 utilization. Several routes for converting CO2 are already known, like the hydrogenation of CO2 into CO (Reverse Water-Gas Shift) and the direct Fischer-Tropsch (FT), producing hydrocarbon

Highlights
CO2 conversion by iron nanoparticles embedded in N-doped carbon. The catalyst surface investigation by DRIFTS during the Fischer Tropsch catalytic tests. The N/C precursor affect the structural parameters of iron catalysts, as showed by XAS experiment. The N-doped catalysts showed a undesirable high selectivity to methane. The promotion of Fe catalysts with potassium did not change significantly

Abstract
Despite many studies aimed on mitigate the CO2, a conversion and selectivity of reactions still need to be improved. This work prepared an iron hybrid catalyst embedded in N-doped carbon for studies in the direct-Fischer-Tropsch reaction. This research investigated the structure properties of catalyst with N-doped carbon and non dopped and their influence on CO2 catalytic performance. At direct FTS (CO2:H2=1:3) conditions, the Fe catalysts showed a considerable CO2 conversion at temperatures higher than 250°C, to C2 –C4 hydrocarbons, methane and mainly CO. It traduces the of RWGS reaction is predominant during the FT synthesis. The N-dopped carbon catalysts showed a higher selectivity to methane probably due to their different strucutural paramenters as showed by high interaction with oxygen/nitrogen detected by EXAFS analysis. The time and the temperature to activated the catalysts under hydrogen atmosphere affect also the activity and selectivity of FTS. The promotion of catalysts with K (Fe/k=0.5) showed a slightly change on selectivity.

Poster session **# Q.13**

Ocean Thermal Energy Conversion Resource Estimation on Deepwater offshore Brazilian

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Keywords
Ocean Thermal Energy Conversion(OTEC); Renewable Energy; CO2 convesion

Impact statement
Owing to the growing concern of the sustainable use of the CO2 in the presalt field, and the need for a clean energy source for hydrogen production through electrolysis. The desalination of seawater through OTEC in a two-stage cycle can offset the need for seawater purification plant for electrolysis of water and as well a clean energy source for hydrogen production.

Highlights
Bathymetry data from the National Oceanic and Atmospheric Administration was analyzed Vector and Raster dataset were obtained using the GIS tools to obtain the thermal gradient Thermal gradients of three buffer zones around the study area were established Two of the buffer zones shows a promising result with slight fluctuation due to season.

Abstract
The goal of the study is to assess the ocean thermal resource along the Santos basin and seek to discover the best sites optimal for OTEC plant deployment. The result will be validated with the output from models developed to determine the ocean thermal resource from any available oceanographic databases. The approach is based on analyzing data from the National Oceanic and Atmospheric Administration using ocean bathymetry data from 2005 to 2017. Raster and vector datasets were obtained via GIS tools to calculate thermal gradient between the surface and selected depths. Thermal gradients were obtained by subtracting sea surface temperature raster from the other selected depths. This process allows for representing areas with thermal gradient equal or greater than 20◦C. Three buffer zones of selected distance was performed on the raster with Santos coast as a reference point to the oil fields located at a distance away from the coast. The historical temperature profile for the 555km (5') buffer zone shows a maximum sea surface temperature of 24oC with a constant thermal difference of 20oC from 950m to 2000m depth. Buffer zone of 1110km (10') with a sea surface temperature of 26oC reveals a thermal difference of 20OC at a depth of 700m and over 22oC at a depth of 1000m and beyond. Thus, this zone can be seen as favourable for OTEC deployment. The maximum thermal difference registered at third buffer zone of 1665km (15') is 24oC, but fairly constant at 20oC between 950m and 1200m depth. Apparently, the three zones of interest would be good option to convert energy throughout the year as there is slight fluctuation due to seasons on the region. However, areas less than 100km to the Santos coast are not suitable for the location of the plant as the maximum thermal difference is 9oC at 1000m depth and is practically impossible for deployment.

Poster session **# Q.14**

Civil and Environmental Liability in CCS activities: scenarios under Brazilian law

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Keywords
Responsibilities; Liabilities; Carbon Capture and Sorage; CCS Rules

Impact statement
Carbon dioxide storage is not provided for by current Brazilian regulation. Parameters are required for the transfer of responsibilities before the operational controls are executed. Defining property rights and securitization mechanisms are important steps in establishing liability rules.

Highlights
'- CCS activities need clear definitions of civil liability for implementation in a jurisdiction - Responsabilities in Environmental Matters are objectives (do not need proof of guilt) in Brazil - Parameters are required for the transfer of responsibilities before the operational controls are executed - Defining property rights and securitization mechanisms are important steps in establishing liabi

Abstract
This article intends to organize and understand the theories and norms related to civil and environmental liability in the Brazilian legal system and its relations with the potential implementation of CCS (Carbon Capture, Transport and Storage) projects in Brazil. Thus, in view of the protection of the environment, safeguarded as a Brazilian constitutional norm and related normative organization, the questions concerning civil and environmental liability are introduced. In addition, international guidelines on the subject in selected country standards are exposed through the composition criteria of the International Energy Agency (IEA) CCS normative repository. Then, notes are made on the fundamental importance of Civil and Environmental Liabilities in the prevention and control of environmental accidents, social risk management and safety in storage and carbon activities, as well as conclusions drawn from the current scenario of Brazilian Environmental Law.

Poster session **# Q.15**

CO2 Conversion into Formic Acid in an Electrolyte System

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Keywords
CO2 Conversion; Formic Acid; Electrolytes System

Impact statement
The study focuses on the proposal of modeling and simulation of an innovative route to obtain formic acid from CO2 conversion in an electrolyte system. While most studies in the literature focuses on promote the reaction by developing novel catalysts with better conversion and selectivity.

Highlights
The electrolyte system was modelled and simulated the intermediates were obtained; The sensibility analysis was carried out obtaining the operating conditions; Low temperatures and high pressures (298 K and 40 bar) favor the production of formate; CO2 conversion is around 80% at 298 K and 50 bar, when the H2O/CO2 ratio is 10.

Abstract
CO2 emissions contribute to the increase in global temperatures and climate changes due to the "greenhouse effect". To reduce CO2 emissions, in principle, there are three possible strategies– reduction of the amount of CO2 produced, storage and use. Among all these alternatives Carbon Dioxide Utilization has gained much attention, since CO2 is abundant and cheap, and can be converted into profitable chemicals. An option to convert this pollutant is to react with hydrogen in the presence of ammonia to transform it into intermediates, such as carbamate and formate, which these compounds are raw material to synthetize many products, such as, methanol, urea and formic acid. The aim of this work is to evaluate the best operating conditions to reach carbamate or formate. The process is an electrolyte system. Chemical and phase equilibria were computed simultaneously to include the effect of the strong interaction between phases and species. The set of reactions to represent the electrolyte system was specified by applying the Chemical Reaction Stoichiometry method. It consists in obtain independent reactions based on the number of components, species and charges. Six independent reactions lead to the products of interest and this set was modelled in the Aspen Plus® process simulator. The thermodynamic model ELECNRTL with Redlich-Kwong Equation of State. A sensitivity analysis was carried out. The results presented that low temperatures and high pressures (298 K and 40 bar) favor the production of formate, obtaining 53% of yield. CO2 conversion is around 80% at 298 K and 50 bar, when the H2O/CO2 ratio is 10.

Poster session **# Q.16**

Systematic assessment of feedstock sources for carbon dioxide conversion by hydrogenation process

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Keywords
carbon dioxide conversion; hydrogen; sustainability

Impact statement
Carbon dioxide hydrogenation is one of the most important methods for the convertion CO2 into valuable products. This work systematicaly evaluates sources of CO2 and H2 to be used in CO2 conversion processes in order to design a sustainable way to convert CO2 into chemicals.

Highlights
A systematic framework to evaluate sources of CO2 and H2 to be used in CO2 conversion processes by direct hydrogenation was proposed. Usage of CO2 from industrial processes with high purity streams is favorable to process economics. Hydrogen recovered from waste streams and produced with renewable electrolysis are the most suitable.

Abstract
Carbon dioxide (CO2) capture and utilization aims to reduce greenhouse gas emissions and dependence on fossil fuels by capturing CO2 and using it as feedstock. Hydrogenation is among the most important reactions to convert CO2 and is a potential opportunity for sustainable process development, being able to produce synthetic fuels and valuable chemicals. As the conversion of CO2 is energy-intensive, assessing the overall process sustainability requires a detailed evaluation of the whole system, starting from the sources of H2 and CO2. Presently, almost all industrial production of hydrogen is based directly or indirectly on fossil fuels, impacting negatively on its environmental loads. Additionally, to capture CO2, conditions such as composition and pressure of the gas stream affects directly on costs and environmental impact of carbon capture. A thorough assessment of CO2 and H2 sources is the first step to design sustainable way to convert CO2 into chemicals. Although a rich literature on CO2 capture and H2 production is available, little attention has been given to the combined assessment of these sources in the context of CO2 conversion. Hence, the objective of this work is to propose a systematic framework to evaluate sources of CO2 and H2 to be used in CO2 conversion processes by direct hydrogenation. Potential sources of CO2 (from power plants to ethanol fermentation) and H2 (from dedicated production to by-product hydrogen) where evaluated considering environmental and economic aspects associated with the usage of each source, the Global Warming Potential and cost of hydrogen/carbon dioxide were used as quantitative indicators; availability and location were used as restrictions. The framework provided an objective selection method to choose appropriate H2 and CO2 sources. Overall, for the CO2, the most promising sources were the emissions from steam reforming of methane, ethylene oxide production and natural gas processing. For H2 sources, hydrogen recovered from petroleum refinery and solar-powered electrolysis are expected to be the most suitable. Still, other aspects must be considered when selecting the proper combination. According to International Energy Agency prospects, H2 production from electrolysis is expected to be more feasible than fossil-fuel based production due to increased technological efficiency and lower renewable electricity prices.

Poster session **# Q.17**

QUANTIFICATION OF CH4/CO2 GAS BUBBLES LEAKAGE USING MULTI-ELEMENT ULTRASOUND IMAGING

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Keywords
Monitoring, Image Processing, Filtering, Sonar

Impact statement
The detection, monitoring and quantification of underwater CO2 leakage is important to ensure the effectiveness of CO2 storage, the public health and the environmental safety and is becoming increasingly important. Moreover as the global warming concern increases there is a need to better characterise gas release mechanisms and amplitudes from natural sources.

Highlights
Sonar images can detect leakages from distances of hundreds of meters. To quantify the leak,the mass and vertical speed of the gas bubbles must be determined. The Finite Element Methodand segmentation algorithms, along with experimental data, are used to calculate the leakage based on the sonar scan.

Abstract
The leakage of greenhouse gases such as CO2 and CH4 (methane) is a serious threat to the environment. From the seafloor, gas escaping underwater originates from the migration of gas through the sediments and diffuses in the water column either asdissolved gas or as a free gas. In the later, this takes theform of bubbles with different sizes and structures varying from small bubble streams to larger bubble clouds. This is the reason why leakages of those gases must be detected, quantified and monitored. With autonomous monitoring devices and autonomous robots, a dynamic asset maintenance and management plan can be deployed with the help of big data technologies and available analytics. In this work the leak detection and quantification is done using sonar technology, which can detect bubbles from a distance of hundreds of meters. The leak quantification using sonar involves multiple technologies, from acoustics and signal processing to fluid dynamics, requiring a careful methodology to integrate the many components. Since each component add some error to the final result must be considered and analyzed. To calculate the amount of gas leakage, the bubble sizes and their spatial distribution will be measured, along with their vertical speed and the relationship between the bubble size and the reflected echo amplitude. Since the bubble sizes cannot be obtained by segmenting a sonar image, because the echoes do not show the entire bubble surface, one solution is to use the amplitude of the received pressure wave to estimate the bubble size. The relationship between bubble size and reflected pressure canbe calculated using available formulas for spherical bubbles. This work will determine experimentally this relationship. Capturing the image of a real bubble, it's size can be estimated using image processing techniques to segment the buble and the recover the bubble contour. This is a required step to find a relationship between the bubble real size and the ultrasound echo amplitude.

Poster session **# Q.18**

Analysis of the inclusion of American LNG as a composition of the Brazilian GN matrix through the Government Program "New Gas Market"

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Keywords
Liquefied Natural Gas, LNG, LNG Brazil, importation LNG

Impact statement
To help the brasilian natural gas sector understand the LNG market as a way to take advantage of its current low prices, composing the supply matrix with other. In addition to competitive pricing, LNG enables the delivery of natural gas to locations not served by the pipeline network and provides for large volumes to be met regardless of pipeline capacity limitations.

Highlights
Opening of the Brazilian gas market from the government program: New Gas Market
Composition of the Brazilian natural gas matrix via importation of American LNG;
Backup option in the supply of large volumes for electricity production and consumption in large Brazilian factories;
Opportunity to acquire natural gas at competitive prices seen in the international market from American shale gas

Abstract
Currently, Brazilian policy has joined efforts to implement the use of natural gas as one of the main elements of energy transition to a low carbon economy. Thus, with the new momentum for the Brazilian natural gas sector, the opening of a single supplier market for the entry of other companies interested in the supply of this energy represents an evolution and generates cost competitiveness, with consequent reduction of prices in the Brazilian market. It is known that the state oil company, Petrobras, is currently responsible for almost 100% of all the natural gas exploration and importation in Brazil. Given this promising gas market development program being instituted by the current federal government, the state-owned company would no longer be the only player for exploration and production of natural gas. The government has instituted a new program called the “New Gas Market”, where Petrobras no longer has the role of sole producer and importer, opening the market to new production agents, as well as being obliged to sell some of its plants and properties, distribution assets and processing units (UPGNs), responsible for processing natural gas. In this way, allowing the acquisition of structures such as transmission and distribution pipelines, as well as regasification terminals by other companies or the possibility of sharing the operation with other companies. This scenario of access and sharing, solves difficulties for companies interested in acquiring and importing LNG in the international market. In this model, the contracts have its price based on the American shale gas, that is very competitive if compared to contracts helded in NBP (National Balancing Point pricing) or JKM (Japan Korea Marker pricing) that have their price benchmarks to international oil. This program will provide an energy transition in the national natural gas sector, where until then Petrobras had been the main supplier since the emergence of the market. The Brazilian government foresees a series of legislative and regulatory changes that will allow the opening of the market, with the evolution of the natural gas sector, generating a new conception of the matrix composed by the importation of Liquified Natural Gas (LNG) and other currently sources (pre and post salt and Bolivian import).

Poster session **# R.01**

Recent studies on health, safety, and environmental impacts in salt Caverns

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Keywords
Salt caverns; Health; Safety; Environment; Carbon capture and storage

Impact statement
Brazil's experience in environmental regulation is relatively new and investments in regulatory capacity will be essential to safe and effective CCS operation. One approach for regulating CCS in Brazil is to develop and implement a pilot regulatory framework for the first demonstrations, which can be revisited prior to wide-scale deployment of the technology.

Highlights
'- The necessity of observing safety issues on the environment and the reduction of these influences have been contemplated. - The recognition of the destructive impacts of the CCS projects has been reviewed. - Salt caverns for separation of carbon dioxide and natural gas have been studied from the perspective of environmental impacts.

Abstract
Regarding the change of global attitude towards efforts to reduce the environmental impact of carbon dioxide, as well as the benefits of new methods in the management of production and transfer and storage of hydrocarbon products, using the capacity of salt caverns for storage of carbon dioxide or natural gas storage has been widely considered. With the implementation of the carbon capture and storage projects, the necessity of observing safety issues and the recognition of the destructive impacts of the CCS projects on the environment and the reduction of these influences have been contemplated. In this work, we propose to study salt caverns used to separate the carbon dioxide and natural gas from the perspective of environmental impacts. This review concentrates on the Health, safety, and environmental issues of deep underground salt caverns used to store hydrocarbons with depths ranging between 800 and 2000 m. Storing carbon dioxide into suitable underground storage is considered the most effective way for a safe and definitive CO2 separation from other hydrocarbons. We will focus on likely pathways of leakage from salt caverns, and a brief explanation of the causes of leakage will be presented based on available articles and surveys.

Poster session **# R.02**

Evaluation of the Potential from the Parana Sedimentary Basin for CO2 geological storage: A case study of the Jorge Lacerda Thermoelectric Complex, Santa Catarina

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Keywords
CCS; Geological Storage of CO2; Paraná Sedimentary Basin

Impact statement
Characterize and understand the potential of CO2 storage in geological units of the Paraná Basin, near the Jorge Lacerda Thermoelectric Complex, in Santa Catarina state, in order to evaluate the geological viability of storing large volumes of CO2 generated in the combustion of coal in the power plants, adapting the energy plants to a reality of lower emissions of greenhouse gases.

Highlights
'- Global scenario of high CO2 atmospheric concentrations; - CCS as an effective alternative for global reduction of CO2 emissions; - Jorge Lacerda Thermoelectric Complex as an important source of CO2 emissions; - Potential from the rocks of the Paraná Sedimentary Basin for geological storage of CO2.

Abstract
The CO2 atmospheric concentration has reached historically unprecedented levels associated with an increase in anthropogenic emissions, mainly from the use of fossil fuels in the last 100 years. Among them, the production of mineral coal related to the energy generation in thermoelectric power plants is one of the most important in the emission of greenhouse gases. Knowing the current global trend of attempting to reduce greenhouse gas emissions, Carbon Capture and Storage (CCS) technology has proven to be an interesting tool for this. It consists of the capture of industrial CO2, compression, transport and injection into reservoirs in geological units, for permanent storage. Thus, the CCS mechanism would be an effective alternative for the global reduction in CO2 atmospheric emissions. However, it is essential to have full knowledge about the characteristics of the reservoir rocks to be used for storage, to ensure that the CO2 will remain in the reservoir for a long time, so as to have a safe use of this alternative without offering other types of social and environmental risks. Thus, the present study aims to evaluate, from available geological information and new mineralogical and organic geochemical analysis, the potential for CO2 storage of the rocks belong to the Paraná Sedimentary Basin, to store the greenhouse gases emitted by the Jorge Lacerda Thermoelectric Complex, the largest in Brazil and Latin America, located in the southeast of the state of Santa Catarina, where are also concentrated a large urban centers and industrial areas considered important emitters of CO2.

Poster session **# R.03**

Possibilities in the Santos Basin for CO2 Geological Storage

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Keywords
Geological Storage, Santos Basin, CCS Possibilities

Impact statement
The Santos Basin is strategic for Brazil, either because it is located near major centers and the Campos Basin, or because it has oil and gas production in ascendency. Looking for possible geological reservoirs in this basin is explained by its growing role in the Brazilian scenario. The present work is a search for reservoirs that are more adequate (in terms of geology and avaiable structure).

Highlights
The analysis of the Santos Basin for CO2 storage is justified by economic factors and its privileged location. The use of depleted oil and gas fields seems an appropriate option for CO2 storage in the Santos Basin. The necessary structure for the venture is in parts available in some fields. Storing CO2 in certain formations of the Santos Basin seems to be a possible endeavor.

Abstract
Carbon Capture and Storage (CCS) technologies are considered a relevant tool for achieving the Paris Agreement goals. The energy sector plays an important role in this paradigm shift, as it accounts for much of the world's total greenhouse gas emissions. Thus, the search for geological reservoirs is essential because it corresponds to a possible final stage of CO2 destination in the CCS chain. In Brazil, the search for reservoirs is also an issue and the analysis of the Santos Basin should not be disregarded. This basin has a privileged location, being close to oil producing and consuming centers. In addition, the presence of local companies that are willing to develop this type of technology is a relevant factor. The search for reservoirs in the Santos Basin revealed that a good storage option would be to use depleted oil and gas fields. The use of decommissioned oil fields still has the advantage of providing economic survival to the site and a new way to deal with the decommissioning phase of projects in their final stages. A good example that fits this situation is the field of Merluza, located about 180km in front of the city of Praia Grande. The Merluza Platform (PMLZ-1) has been in operation since 1993 and produces the Merluza and Lobster natural gas fields. Ilhabela reservoirs can be understood as examples of abnormally high porosity at their depths, averaging 21% in well 1-SPS-20. The reservoirs of the Juréia Formation base, on the other hand, have an average porosity of 12% in well 1-SPS-25, which is relatively lower than Ilhabela Member's porosity. The fact that it is a deactivating gas field favors numerous advantages: greater data availability, knowledge that the structure (if unaffected) is capable of holding gas, the presence of a gas transport infrastructure, among others. More detailed study of features (from geological to economic possibilities) is needed to be able to actively state that the Merluza field is suitable for the development of a carbon storage project. However, looking at this field and all its capacity is already an indication that the Santos Basin can be used for more ambitious CCS projects.

Poster session **# R.04**

Enhancing the geological evaluation of CCS potential with Data Science: A case study of the Parana Basin

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Keywords
CCS, Data Science, Geological Evaluation

Impact statement
All-out geological data integration is key for CCS potential evaluation, Data Science offers to drive the best outcomes.

Highlights
'- Data Science delivers solutions to problems where our theoretical knowledge is still incomplete - Effectively integrating all the available geological data to improve reservoir models - Using Machine Learning algorithms to evaluate the CCS potential of the Paraná Basin

Abstract
This works aims to explain the benefits of using Data Science for evaluations of CCS potential since traditional methods do not offer a complete geological data integration and intends to contribute to strength the relationship between the academic research and the private sector. Furthermore, using a case study from the Irati Formation, this work analyses relationships among the available geological data by using Machine Learning algorithms as a tool to understand the CCS potential of the Parana Basin and seeks to extract insights that help increase the accuracy of reservoir models during the exploration phase and therefore to enhance CCS project assessments.

Poster session **# R.05**

Lipid production by Didymogenes sp.: a microalgae isolated from mangrove

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Keywords
bioconversion, carbon dioxide, microalgae

Impact statement
Possibility of microalgae to use CO2 during the photosynthesis process and to stock products with high value, as biodiesel. Convert CO2 in lipids by biotechnological process with microalgae from mangrove

Highlights
Microalgae isolated from mangrove was identified as Didymogenes sp; Lipid production on nitrogen deprivation

Abstract
One natural way to recycle the CO2 is photosynthesis. The ability of microalgae to fix CO2 is 10 times greater than of terrestrial plants. The majority microalgae species can grow on aquatic environmental and tolerate different CO2 concentration, being considered as good candidates for CO2 mitigation. Under extreme environmental conditions, microalgae grow under stress, synthesizing and producing various secondary metabolites. In recent years, the research with microalgae (including cyanobacteria) are receiving significant attention as a viable feedstock for the production high values molecules, like biodiesel. In this sense, the aim of this study was to convert CO2 in lipids by microalgae. A microalgae isolated from mangrove was identified as 95% of Didymogenes sp. and tested to produce lipid under stress conditions. The first test was bubbling air atmosphere in three different condition using BG 11 medium in bottles of 250 mL. The conditions were: a) control (complete culture medium), b) culture medium without nitrogen and c) culture medium without nitrogen plus acetate (4%). To verify the presence of lipid, a colorant Nile red (NR) was used and scanned by spectrofluorimeter. The previously results with NR revealed a peak (confirming production of lipid) in both cases of stress, but in the microalgae grown in a presence of acetate, the peak was bigger than in other condition (without acetate). Through the analysis of Fm/Fv (to check the efficiency of chlorophyll) it was possible to confirm that microalgae grew with acetate was in a higher cellular stress, what could be a reason for more lipids production. The next steps are: to perform more lipid-analysis and increase the CO2 supply.

Poster session **# R.06**

Numerical simulation of an axisymmetric incompressible ejector

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Keywords
CFD; Optimization; Ejector

Impact statement
The ejectors show up as a promising device to recover energy from low-grade pressure sources, being able to work as a compressor or vacuum pump. The approach to reduce the concentration of CO2 in the atmosphere known as carbon capture and storage (CCS) is an example of process that can take advantage of the use of ejectors with high efficiency.

Highlights
Simulation of an incompressible ejector using COMSOL Multiphysics® ; Validations of these simulations with the literature; Comparison of the simulations; and Optimization of the k-epsilon model.

Abstract
The recent increase in the environmental awareness about the impact of human activities creates a field of great interest to the scientific community, hence, the focus of several researches. The ejectors show up as a promising device to recover energy from low-grade pressure sources, being able to work as a compressor or vacuum pump. Although ejectors have advantages like low maintenance cost, no moving parts, high reliability and low installation cost, they have low efficiency when compared with other devices quoted above. The approach to reduce the concentration of CO2 in the atmosphere known as carbon capture and storage (CCS) is an example of process that can take advantage of the use of ejectors with high efficiency. The present work investigates the flow features of a simple as possible ejector, that is, an incompressible and monophasic ejector. The simulated geometry was built using the dimensions of experimental tested geometries, allowing the validation of the numerical results with experimental data. The software chosen was the COMSOL Multiphysics® that uses the finite element discretization scheme. Because of the complexity of the flow, the simulations were performed using the Reynolds averaged Navier Stokes equations (RANS), thus, it is assumed that the flow is turbulent everywhere in the domain. The turbulence models required to solve the closure problem used in this paper were: k-ε, k-ω and k-ω SST. The wall treatment employed in the models k-ε and k-ω was wall function and low Reynolds for k-ω SST model; boundary conditions were set up as reported in experimental data. With the purpose of reducing the discretization error, the sensitivity analysis was carried out using a methodology presented in the literature. The simulations point out that the k-ε and k-ω SST turbulence models have a very good agreement with the experimental result up to the efficiency peak. However, for points beyond this peak, one can observe that the k-ε and k-ω SST models overestimate the efficiency coefficient. To enhance the results of k-ε model, an optimization routine was carried out at the closure constants of this model. Despite enhancements in the capability of the model k-epsilon in predicting the performance of the ejector, further experimental data will need to be performed to better understand the flow field behavior in order to validate the enhanced model.

Poster session **# R.07**

Nucleation rate calculation in supersonic nozzles.

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Keywords
Condensation, cubic EoS, supersonic nozzles.

Impact statement
The condensation proccess in supersonic nozzles have been object of several thermodynamic and computational fluid dynamic researches because occurs in many technical applications such as supersonic separarators and machinary operating with steam and nuclear reactors.

Highlights
Implementation of the improved Peng-Robinson with the Strjek-Vera modification equation-of state in a quasi-one-dimensional model in to calculate the flow behavior and the nucleation rate during an isentropic expansion of steam at low pressures.

Abstract
The condensation process in supersonic nozzles has been the focus of many thermodynamic and computational fluid dynamic researches since occurs in many technical applications, such as supersonic separators and machinery operating with steam and nuclear reactors. The present work is focused on the calculation of the nucleation rate based on the classical nucleation theory as an initial approach to characterize the liquid phase formation in supersonic nozzles. The analytical modelling of an isentropic expansion which will leads to non-equilibrium condensation of steam at low pressures is carried out in a quasi-one- dimensional model. The complete thermodynamic model of the improved Peng-Robinson with the Stryjek-Vera equation-of-state is built using the high-level programming language Python. Algebraic equations of the mass, energy and momentum conservation are solved and coupled to the correlations provided by the fundamentals of the homogeneous nucleation. The results have a good agreement with the experimental and numerical data available on the reviewed literature.

Poster session **# R.08**

Numerical investigation of supersonic nozzle for gas separation

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Keywords
Computational Fluid Dynamics (CFD), Supersonic gas separation, shock wave

Impact statement
The design of a gas separation system prototype is one of the main goals of Project 39. The use of CFD (Computation Fluid Dynamics) is paramount to the development and optimization of the separation system design. In spite of that, due to complexity of the flow inside the separator device, a good prediction of the flow by CFD is quite challenging and it is applied for three configurations.

Highlights
'- CFD codes based on the Finite Volume method have been applied to simulate the flow through a supersonic gas separator. - A Shock train flow pattern was observed at the diffuser of the supersonic gas separator. - Boundary layer separation was noted downstream the shock waves.

Abstract
The proposed work is under the scope of the RCGI project 39 (Development of gas supersonic separator – optimization, numerical and experiments), with a main goal to design and develop a supersonic separator prototype. Such a device is applied to separate heavier components from the natural gas, such as carbon dioxide. In this context, the CFD (Computational Fluid Dynamics) tool is used to predict numerically the flow behavior of different configurations of supersonic nozzles as the main part of the gas separation system device. Such numerical results provided by CFD allow a better understanding and prediction, as well as optimization, of the flow behavior inside the supersonic separator device. For this work, three main supersonic nozzle configurations were considered. The first configuration is the Arina's geometry, which is a simple convergent-divergent supersonic nozzle with a normal shock wave (pressure ratio of 1.2). The second configuration is a supersonic nozzle that has a long straight section followed by a diffuser. At the straight section, a collector is installed to capture and separate the condensed heavier components from the rest of the gas. The third configuration is named as Papamoschou's geometry, which is also a convergent-divergent nozzle, with respect to the Arina's geometry, however with a higher NPR (Nozzle pressure ratio) of 1.4. Such a configuration was used to evaluate the capability of the CFD solver to well predict the flow behavior inside the supersonic nozzle as experimental results are available for comparison. The CFD results for the Arina's geometry, using the ANSYS Fluent code (finite volume method), showed that the predicted flow field is in accordance with the expected flow physics of a supersonic convergent-divergent nozzle with the presence of a normal shock wave. For the second configuration, by using the CFD++ code (finite volume method), the simulations revealed at the diffuser a shock wave with a shock train pattern. In addition, this geometry is modified with a collector device installed at the straight section part. Besides a main shock wave at diffuser section as previously observed, the results showed the presence of an oblique shock wave at the collector inlet followed by boundary layer separation. For the third configuration, the flow pattern of the shock wave and its position predicted by the CFD solver (ANSYS Fluent) were in good agreement with the corresponding experimental results.

Poster session **# R.09**

Thermal behavior of interfacial fluid slip

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Keywords
molecular dynamics, fluid-solid interfaces, slip length

Impact statement
This study is aimed at the development of material-specific boundary conditions meant to be implemented in multiscale fluid simulations; once the analysis is extended to more complex substances, it may help in the optimization of nanostructured membranes designed for natural gas separation in carbon capture processes.

Highlights
• Universal behavior is observed for the slip length as a function of temperature. • The proposed heuristic model is capable of describing qualitatively different thermal behaviors. • For a certain range of interface parameters, the slip length increases by many orders of magnitude at low temperatures.

Abstract
The relation between fluid slip on a solid surface and flow temperature is investigated with the help of molecular dynamics simulations. An atomistic Couette configuration, consisting of a Lennard-Jones fluid and rigid walls, is prepared and evolved to its steady state, where the slip length can be readily extracted from the linear velocity profile. Simulations are carried out for a broad range of temperatures and for different magnitudes of the fluid-solid chemical affinity. This last quantity is found to affect the overall shape of the slip length vs. temperature curve. Depending on its value, three distinct types of thermal behavior are observed, all of which are well described by a simple heuristic function whose adjustable parameters have a clear physical interpretation. We discuss the significance of our results as regards multiscale simulations with material-specific boundary conditions.

Poster session **# R.10**

RCGI Sustainability Matrix: assessing R&D projects in light of the Sustainable Development Goals

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Keywords
Sustainable Development Goals; United Nations; Sustainability assessment

Impact statement
A new method is being developed to assess the RCGI project in light of the United Nations Sustainable Development Goals. We aim to build a matrix characterizing our R&D projects regarding their impact on sustainable development.

Poster session **# R.11**

Direct Alkaline Anion-Exchange Membrane Fuel Cell to Converting Methane into Methanol

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Keywords
methane to methanol, methane oxidation, electrocatalysts

Impact statement
Alkaline fuel cell to convert methane in electric power and higher value-added chemicals cogeneration

Highlights
Methane in electric power and metanol on Pt/C, Pd/C and Ni/C
Alkaline Anion-Exchange Membrane Fuel Cell for energy and chemical cogeneration
In Pt/C presents power two times higher than other materials and 20¨% of conversion of methane to methanol

Abstract
Methane is the main constituent of natural gas and can be converted in energy with fuel cell application and higher value-added chemicals cogeneration. In Alkaline Anion-Exchange Membrane Fuel Cell (AAEMFC) is possible led in a way that leads to more oxidized products, therefore more electrons transferred. The investigation was realized for the methane oxidation on Pt/C, Pd/C, Ni/C as catalysts. The electrocatalysts were prepared using a sodium borohydride method with 20 wt% of metals loading on carbon. The X-ray diffraction (XRD) analysis revealed a cubic face-centred structure (CFC) for Pt/C and Pd/C catalysts, was observed Ni/NiO phases for Ni/C electrocatalyst. The Transmission Electron Microscopy (TEM) exhibited a good dispersion of nanoparticles and some agglomerations on the support, with a mean size of 6.4 nm for Pd/C, 5.7 nm for Ni/C and near to 2 nm size for Pt/C. The experiments with AAEMFC showed that all materials can carry out the reaction spontaneously. Pt/C catalyst presents energy density twice times higher than the other materials. FTIR data suggest that methane was converted into small products organic molecules such as methanol and formate in different potentials for Pt/C, Pd/C, and Ni/C.

Poster session **# R.12**

CO2 INJECTION MONITORING METHODS IN OFFSHORE GEOLOGICAL WAREHOUSE

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Keywords
Monitoring, CO2 injection, Geological storage of CO2

Impact statement
Society requires productive changes and reduced impacts, with geological storage of CO2 being an alternative. So the problem is: What monitoring methods are suitable for injection for offshore geological storage of CO2?

Highlights
Investigation of the environmental impacts of brine disposal in an offshore environment is established as a research problem to the question of how brine disposal and treatment are carried out in the case of salt formation in offshore environment which can cause significant environmental degradation, which can be mitigated by appropriate measures.

Abstract
Brine can be harmful to the environment due to its salinity, temperature and toxic substances, which are directly dependent on the cave leaching process for CO2 storage.
The salinity of the brine produced by desalination is about 60 ppt, the oilfield mining 100 ppt, the salt dome mining is 250 ppt and the potassium mining 350 ppt, and its temperature production is very high, between 90ºC and 115ºC. Increased salinity disrupts the osmotic balance of marine species and the environment, resulting in cell dehydration, decreased cell wall pressure, and can lead to the death of several species.
The high temperature of the brine has harmful effects on marine life as the toxicity of metals and chemicals increases with temperature while oxygen solubility decreases, resulting in lower levels of dissolved oxygen in the receiving marine environment.
Small temperature variations (1ºC) can, if they last, significantly alter the composition of the local ecosystem and, although marine organisms may temporarily adapt to small temperature changes, they are unable to maintain it permanently and prolonged exposure to the environment may occur. post-change environment in the long run be fatal to marine life.
Selecting an appropriate brine disposal method to meet existing environmental regulations plays an important role in the viability of industries producing this effluent. In addition, accommodating future environmental regulations is also an important planning issue for any venture, making knowledge of brine environmental regulations useful in providing general principles and pertinent information about current and future regulatory trends, Just as understanding available disposal methods is also helpful in choosing appropriate disposal systems that are environmentally, economically and technically feasible to locate.
Brine is produced in various quantities, so understanding its characteristics and its impact on the environment is important for developing and implementing appropriate environmental policies by environmental protection agencies and other responsible agencies.

Poster session **# R.13**

Environmental impacts limited to waste disposal in offshore environment

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Keywords
Environmental impacts. Brine disposal. Geological storage of CO2.

Impact statement
Brine is the leading product of cave construction leaching for offshore geological storage of CO2 and many other processes. In recent decades brine production has increased due to the rapid increase in various processes.

Highlights
The general principles of law are basic and general directives guiding the interpreter applying the right in case of omission of the legal text.
Many principles in the right of the International agreements.
The Kyoto protocol and the Paris Agreement shall be an increasingly clear sense of development based on environmental protection and the reversal of the effects of greenhouse gas emissio

Abstract
The present work proposes a reflection on principles applicable to Carbon Capture and Storage (CCS), within the perspective of Constitutionalization of Law and considering the intersection between Environmental Law and Economic Law and the hermeneutic process of integration of legal norms. The method used was the deductive, starting from the general principles of the law for the principles of law related to the activities of Carbon Capture and Storage, through interpretative technique and bibliographic and documentary analysis.

Poster session **# R.14**

Carbon Storage and its property rights in the Brazilian legal system

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Keywords
Property Right, CCS, Energy Transition

Impact statement
Property interests can play a role in defining the geologic storage costs through the purchase of necessary geologic reservoir property rights and the value of storage through ownership of injected carbon dioxide, as well as have impact on the definitions of liabilities. Liabilities can represent a significant cost given that it represent an economic risks.

Highlights
The definition of property rights impact on liabilities predictions
Liabilities represents economic risks
There is a lack of regulation in terms of property rights of pore-space

Abstract
The technology, known as carbon capture and sequestration (CCS), involves capturing CO2 from a stationary source and injecting it into a suitable storage location. Among the storage possibilities. The use of geological formations as captured carbon dioxide storage reservoirs has been received more attention as a feasible large scale site. Potential geological reservoirs include oil and gas fields, and geological formation. In that sense, CCS storage operators must be able to access millions of acres of deep subsurface "pore space" roughly a kilometer below the earth's surface to sequester the CO2 for hundreds to thousands of years. This Article studies a full range of property rights relating to ownership of subsurface pore space, accordingly to Brazilian current legal framework. The main question is: Who does the captured CO2 belong to if stored in geological Reservoir? In order to do that, the first part presents the general delimitations of property rights in the Brazilian legal system, then briefly exposes the trajectory of the distinction among general land ownership and the underground ownership. Finally, the current legal prediction about CO2 and pore space property rights. Lastly, final considerations are presented. The difficulty of the question lies in the fact that the Brazilian Federal Constitution exceptionally emphasizes as mineral property found in the Union, which could indicate that the property of CO2 stored underground would be transferred to Federal Government. On the other hand, the definitions of existing property rights refer to pre-existing underground resources, potentially extractable, and not to what could be “injected”. In that case, there is an absence of specific legislation. Given the constitutional determinations, it can be stated with relative conviction that there is a huge “gray zone” over the property rights of CO2 injected permanently in geological formation. This scenario demonstrates the legal and regulatory lack on CCS activities in Brazil legal system and corroborates to the identified need for in-depth studies and edition of robust legislation issues to ensure the necessary conditions for the implementation of this technology in Brazil.

Poster session **# R.15**

PHB production optimization by isolated Methylopila oligotropha from mangrove

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Keywords
PHB, Methylopila oligotropha, Mass Spectrometer

Impact statement
Focusing on fast growing and high PHB/dry mass yield we are testing different conditions to achieve high density of cell and more PHB per batch using a bacterium from Methylopila genus which PHB production potential is still poorly known. This bacterium was identified using a new method based on mass spectrometer developed in this project.

Highlights
Identification of bacteria able to produce PHB using one colony based on mass spectrometer Study of Methylopila oligotropha PHB production potential High yield PHB production Identification of best parameters for PHB production in bioreactor experiments

Abstract
The methylotrophs bacteria can use methane and methanol as carbon sources to produce biopolymers including the polyhydroxybutyrate (PHB) a very promised substitute for the environment contaminant oil-derived polypropylene. This kind of bacteria can be very effective to help to decrease PHB price production and promote its use in substitution of several environment contaminant plastics. The search for methylotroph bacteria able to produce PHB is a very arduous job being necessary to grow all isolates and submit all of them to extraction processes and product characterization. Looking for time reducing and optimization of resources, we tested the Matrix Assisted Laser Desorption/Ionization technique (MALDI-Biotyper) to identify polymer producer bacteria based on a single isolated colony with success. Based on this method, we selected the Methylopila oligotropha isolated from mangrove to study the potential of this bacterium to produce high yields of PHB in controlled conditions. We could stimulate the cell production up to 40 mg per liter of medium achieving 25% of PHB accumulation.

Poster session **# R.16**

Hyperbranched polyesters based on bis-MPA a novel strategy for one-pot green synthesis in supercritical CO2.

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Keywords
Hyperbranched polymers, bis-MPA, supercritical CO2.

Impact statement
This new synthetic method, pseudo-one-pot supercritical CO2 acid catalyzed synthesis, to obtain hyperbranched polyesters will allow a more sustainable approach to new catalysts for CO2 valorization and new phase behavior modifiers based on these materials.

Highlights
Clean synthesis of Poly-hyper- (bis-MPA) in supercritical CO2. Characterization and synthesis of hyperbranched polymers in supercritical CO2 for applications as catalysts and phase behaviour modifiers.

Abstract
The properties of polymers are directly dependent on their structure. A kind of architecture that has been drawing much attention is the hyperbranched polymers, which are polymers with structure as highly branched as possible. Due to their unique characteristics, these polymers are attracting great interest in areas suchas drug delivery and catalysts support. The present work will study the synthesis of polyester-type hyperbranched polymers, formed by AB2 type monomers (one acyl group and two hydroxyl groups). The synthesis was carried out by the transesterification of the esters derived from 2,2-Bis(hydroxymethyl)propionic acid (bis-MPA), using supercritical carbon dioxide (scCO2) as reactional medium, which is a green, solvent free method. First, the starting material Trimethylolpropane (TMP) (or similar alcohols) and the acid catalyst (p-Toluenesulfonic acid, or similar) were added to the reactor, then the system was pressurized to supercritical conditions (above 100 °C and 150 bar of CO2). After that, to obtain the higher possible branching, the ester was added gradually to the reactor. To move the equilibrium toward the polyester formation, the alcohol formed from the transesterification of the ester was removed via a controlled scCO2 flow through the system. The resulting polymer was the Poly-hyper-(bis-MPA). The product was characterized by nuclear magnetic resonance (NMR), which showed the formation characteristic peaks of the different polyester groups. The degree of branching was characterized by mass spectrometry (MALDI-TOF MS). The next step of the work will be the functionalization of the synthetized Poly-hyper-(bis-MPA) with CO2-philic group, in order to obtain polymers with more affinity with CO2. Acknowledgments: IQ-USP, EP-USP, RCGI, Shell, FUSP.

Poster session **# R.17**

Performance of Devito on HPC-Optimised ARM Processors

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Keywords
High performance computing, Finite differences method

Impact statement
With Devito, Arm based processors are capable of delivering performance similar to state-of-the-art Intel Xeon processors for the execution of seismic inverse problems.

Highlights
Devito is shown to be capable of generating efficient high performance code for Arm processor. All models compiled and ran successfully. No architecture specific code tuning was necessary to obtain high performance other than sepecifying the compiler and its options.

Abstract
We evaluate the performance of Devito, a domain specific language(DSL) for finite differences on Arm ThunderX2 processors. Experiments with two common seismic computational kernels demonstrate that Arm processors can deliver competitive performance compared to other Intel Xeon processor.

Poster session **# R.18**

Numerical investigation of low pressure non-equilibrium condensation of wet steam in a converging-diverging nozzle

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Keywords
Condensatiom, non-equilibrium, metastability

Impact statement
Our research group has been investigating the physical models that describe the condensation phenomena and we have been able to successfully simulate the presence of the condensation wave in high-speed wet steam flows for low pressures.

Highlights
Non-equilibrium condensation for low pressures. High-speed flows of wet steam. Condensation wave position. Changes in pressure along the nozzle due to condensation.

Abstract
A numerical investigation into non-equilibrium condensation of wet steam flow through a convergent-divergent nozzle was conducted . The physical model for condensation is based on the classical nucleation theory (CNT) and the fluid model for the gaseous phase is the Peng-Robinson Stryjek Vera equation of state. In accordance with the experimental results, the simulations successfully reproduce the presence of a condensation wave. In our analysis we have investigated both the presence of condensation waves in high-speed wet steam flows and how the position of such waves change with different inlet pressures and temperatures, in a low pressure range.

Poster session **# S.01**

Computational analysis of high-order continuous Galerkin implementation of the acoustic wave equation

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Keywords
Acoustic wave equation;
Continuous Galerkin;
Computational analysis

Impact statement
In order to reduce the computational cost of Full Waveform Inversion in seismic imaging we can decrease the cost of the forward problem. Since high accuracy is needed this study compares the computational efficiency of different orders and mesh sizes for a Finite Element Method implementation.

Highlights

- Using high-order Continuous Galerkin methods it's possible to reduce the computational cost in the forward acoustic wave problem.
- Different orders of the nodal Continuous Galerkin method were implemented on various mesh sizes to analyze h and p convergence.

Abstract
Numerical methods are used in a considerable number of fields to model a variety of physical processes providing accurate solutions. One of these physical processes, acoustic wave propagation, is used in Seismic Imaging. In order to create an accurate image of Earth's subsurface, methods such as Full Waveform Inversion are used. This is an iterative method; whose computational cost also depends on the forward model. This study initially focuses on reducing the computational cost of the forward model, while maintaining or increasing the accuracy, by using high-order finite element methods. The present project studies Continuous Galerkin methods, implemented in the Firedrake framework. The Firedrake project uses the Unified Form Language (UFL), a domain specific language (DSL), developed by the FEniCS project enabling quick implementation of equations and models since it closely resembles mathematical notation. This software is used in modelling different order implementations of the nodal Continuous Galerkin method. The computational cost for obtaining the same errors using different orders and different mesh discretizations in a structured triangular mesh is calculated. The results show that using higher-order basis functions on the finite element Continuous Galerkin method it is possible to reduce computational cost in the forward acoustic wave problem in a structured mesh.

Poster session **# S.02**

High-order discontinuous Galerkin method for acoustic and elastic wave equations

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Keywords
high-order; discontinuous Galerkin; wave propagation

Impact statement
This work intends to contribute to the development of computational tools for seismic imaging and inversion.

Highlights
'- Numerical simulations of the acoustic and elastic wave equations. - High-order numerical method. - Interior penalty discontinuous Galerkin method. - Newmark time-stepping scheme

Abstract
In computational geophysics, numerical simulation of wave propagation in the earth's interior is an important research topic and has been extensively investigated in the last four decades, due to the challenging physical obstacles, which involve three-dimensional domains with heterogeneous materials, discontinuities between interfaces and complex geometries. In the present work, we study the second-order acoustic and elastic wave equations by means of numerical simulations. High-order finite element method was used and the discontinuous Galerkin approach was employed for the spatial discretization. We chose the interior penalty discontinuous Galerkin method to perform the numerical simulations, due to wide acceptance by the scientific community and for being a well-established numerical method to deal with wave problems. For the time discretization, we applied the Newmark time-stepping scheme, which is a second-order scheme in time. Convergence analyses were carried out in order to evaluate the performance of our methodology. Firedrake was the finite element framework adopted to develop the numerical analysis, which is a modern environment to deal with partial differential equations.

Poster session **# S.03**

Mechanistic studies of CO2 reduction to hydrogenation using homogenous catalysis

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Keywords
CO2, alcohols, homogeneous catalysis

Impact statement
Hydrogenation of CO2 to higher alcohols without additives; Hydrogenation of CO2 to butanol at low temperature.

Highlights
Hydrogenation of CO2; Hydrogenation of CO2 at low temperature; Hydrogenation of CO2 to higher alcohols.

Abstract
Control of the constant emission of greenhouse gases is one of the greatest challenges of mankind. Among the gases that cause greenhouse effect, CO2 stands out. Therefore, several strategies to sequester CO2 from the atmosphere are being studied, among them, the transformation of CO2 into valuable products such as ethanol and acetic acid has been pointed as promising solution to this issue. In the present work the reduction of CO2 to ethanol and/ or carboxylic acids has been carried out at high pressure and low temperature. T.The study of the effect of H2O on the reduction and CO2 to ethanol was studied from 0 to 25% H2O. The reaction selectivity depends on the amount of water presented in the reaction medium. Moreover, the mechanism of CO2 reduction is currently being studied by DFT theoretical calculations and mass spectrometry.

Poster session **# S.04**

Carbon dioxide (CO2) emissions and their impacts on the production of fossil fuels in the Brazilian geological presalt

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Keywords
emerging technology; geological presalt; carbon dioxide

Impact statement
Demand for natural gas appears to be increasing in the ten-year energy expansion plan. Therefore, geological presalt is an important source of this resource, but to explore it some technological alternatives must be considered for the associated high carbon dioxide levels are not emitted into the atmosphere.

Highlights
Brazilian geological Presalt is an important reservoir of Brazilian natural gas, however, it is associated with a large amount of associated carbon dioxide. With further development of these fields to meet natural gas demand, new CO2 mitigation technologies need to be implemented. Therefore carbon capture and storage (CCS) is an important alternative.

Abstract
Climate change is one of the most recurring and important issues for the world's major agendas and agreements today, including more recent actions such as the Paris Agreement and the seventeen sustainable development goals (mainly 7 and 13, associated with clean energy generation). and action against global climate change) both drafted in 2015. One of the main causes is the emission of greenhouse gases, especially carbon dioxide (CO2). This gas can come from various sources, but in this paper the focus of the study is related to the emission from the production of one of Brazil's main oil and natural gas reservoirs, the Pre-Salt. It is found on the southeastern coast of Brazil and associated natural gas has a high concentration of mixed carbon dioxide (CO2). In order to balance the increase in production - already observed since 2011, when the exploration began - the growing demand for gas from the future perspectives of energy planning and the goals set by Brazil under the Paris agreement, the emerging dioxide capture technology. Carbon dioxide through membranes and the storage of this gas, which are already in use, will have to intensify in the offshore fields for natural gas production that does not exceed the limits of sustainability.

Poster session **# S.05**

Operation and decommissioning of storage facilities for CCS activities in Brazil

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Keywords
Carbon Capture and Storage; Operation and Closing of Facilities; Monitoring and inspection; Technical requirements; Legal and Operational

Impact statement
The theme aims to explore the technical, legal and operational aspects of CCS storage facilities from project design to post-development or decommissioning. The focus will be on the gas storage phase, specifically the verification of the location and authorization of storage activities, operation of these facilities, responsibility during the project period and authorization for decommissionin.

Highlights
'- Lease Verification and Storage Activities Authorization - Responsibility during the project period - Carbon storage and Monitoring, Reporting and Verification Requirements - The legal environment - Storage Location Closure Authorization

Abstract
Knowledge of the scope of the project to be developed is one of the pillars for its successful execution, especially when it is a robust and relevant project, with several interfaces, stakeholders, technical complexity, high investment, wide applicable legislation, especially with regard to to the environmental area. In the meantime, before starting the execution of the project, it is necessary, among other aspects, to study its technical feasibility, as well as the legal environment to which it will be submitted, in order to anticipate setbacks and avoid unnecessary financial expenses. During the project period, the operator is responsible for any liability for damage caused by the project, such as damage to the environment, human health, other resources or damage to third party assets, as well as the cost of remedial action necessary to limit the extent of the project. damage and the cost of damage-related remediation measures that can have impacts with local, regional and global effects. Monitoring, Reporting and Verification (MRV) issues are prominent in international CCS-related legislation, with definitions of methodology for obtaining operations licensing and how site owners and operators should manage such operations, also specifying periodicity and characteristics. minimum reporting techniques for tracking activities. With respect to closure, international best practices should be followed with at least a buffering and abandonment procedure including removal of tubing and wrapper, sealing of the formation with a fluid to reduce its permeability, placement of cement plugs or other insulation material. and test plugs. In relation to Brazil, the sedimentary basins of Paraná, Campos, Santos, Potiguar and Recôncavo are classified as those with the highest prospect for CO2 storage in Brazil, mainly due to the outstanding hydrocarbon production and the presence of mature fields. Paraná Basin, the occurrence of coal deposits. In addition, these basins have a good association between sources and sinks, and CO2 transport pipeline network, which increases their prospectivity. Emissions from sources within these basins (up to 300 km) reach around 368 Mt / year, and the Campos Basin with the largest theoretical capacity for storing CO2 in oil fields with estimated theoretical capacity of 950 Mt CO2. , which would be sufficient to store the equivalent of 3.5 years of total emissions from Brazilian stationary sources.

Poster session **# S.06**

Electrocatalytic oxidation of Methane in an acidic electrolyte using PdMn/C-ITO electrocatalysts synthetized by sodium borohydride reduction Process

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Keywords
PdMn/C-ITO electrocatalysts, Electrochemical Oxidation of Methane, Acid Medium, Sodium Borohydride Reduction Process

Impact statement
This work aims at critical issues concerning some of the main technological and scientific challenges towards the use of natural gas in fuel cells.

Highlights
The research topics are focused in a technology: proton exchange membrane fuel cell (PEMFC). The main topics to be studied are: a) anodes for efficient electro-oxidation of methane; b) membranes for high-temperature PEMFC; c) high performance electrochemical catalysts for methane oxidation for the electricity generation and products of high value trades.

Abstract
Pd/C-ITO and PdMn/C-ITO electrocatalysts with different atomic ratio (90:10, 70:30 and 50:50) were synthetized by borohydride reduction method and characterized by X-ray diffraction, Transmission electronic microscopy and electrochemical studies (cyclic voltammetry). The electrochemical studies showed that PdMn(50:50)/C-ITO had superior performance for electrochemical oxidation of methane in an acidic electrolyte at 25 oC compared to others electrocatalysts prepared. The experiments in a single DMEFC also showed that the PdMn(70:30)/C-ITO electrocatalyst exhibited higher performance for methane oxidation in comparison with Pd/C-ITO, PdMn(90:10)/C-ITO and PdMn(50:50)/C-ITO electrocatalysts. These result indicated that the addition of Mn to Pd favor the electrochemical oxidation of Methane in acid medium, where this effect could be attributed to the synergy between the constituents of the binary electrocatalysts or to electronic modification of Pd atoms by the neighboring Mn atoms as the proximity of Pd and Mn atoms on the surface of the C-ITO (bifunctional mechanism - the presence of Pd and Mn oxides species).

Poster session **# S.07**

Analysis of natural gas reforming to hydrogen production in association with CCS and carbon market in the Pre-Salt region

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Keywords
Hydrogen, Natural gas, CCS

Impact statement
This study is innovative because it considers applying CCS and credits obtained from carbon market in the process of hydrogen production from natural gas (NG) reforming. Additionally, it contributes to increase the natural gas demand coming from the Pre-Salt area via hydrogen production.

Highlights
• H2 is a major substance used in the production of several compounds and it could provide energy storage • NG reforming is a way to obtain H2 whose process is less expensive, but this process has emissions • This study aims to analyse if H2 production from NG reforming with CCS and credits obtained from carbon market can be environmentally and economic advantageous • H2 production from Pre-Salt

Abstract
Molecular hydrogen (H2) is widely used in the chemical and petrochemical industries. This substance is used to produce various compounds and is considered to be used as a source of clean energy. H2 is the main input for removing sulfur from various fuels such as gasoline and diesel in refineries. Due to increasingly stringent environmental legislation, the demand for hydrogen is increasing. Hydrogen can also be used to produce electricity through fuel cells. Hydrogen has the potential to be a fuel with low greenhouse gas emissions. In its combustion, the main product is water and the only resulting pollutant is nitrogen oxide (NOx). The use of catalytic burners allows NOx emissions to be reduced to low levels. Most of the time, hydrogen is found in nature associated with other chemical elements like water or hydrocarbons. Its production is possible through the application of specific processes. Hydrogen can be obtained from water electrolysis, in which the electricity required for the process can be supplied from renewable sources. Natural gas reforming is the most economical route to hydrogen production, as the raw material is easily obtainable and can be found at competitive costs. The supply of large amounts of clean hydrogen could enable a strongly renewable energy system in the future. Hydrogen can also contribute to the security of power systems with high participation from variable renewable sources. Hydrogen produced by natural gas reforming is not considered as sustainable as hydrogen obtained by water electrolysis. It´s because natural gas reform emits carbon dioxide. The use of technologies such as carbon, capture and storage (CCS) can boost the production of clean H2 by natural gas reform. Although the use of CCS in hydrogen production makes this route less economically competitive. One solution to this loss of competitiveness would be to obtain additional revenues in a carbon market for the production of clean hydrogen. Any additional revenues from a carbon market could give more competitiveness to hydrogen produced by reforming of natural gas associated with CCS. In this context, it is possible to consider hydrogen production through the abundant natural gas present in the Pre-Salt region. This sustainable hydrogen production would be an important way to increase the demand for pre-salt natural gas.

Poster session **# S.08**

REGULATION OF PIPED GAS DISTRIBUTION AND MARKETING ASPECTS (SELF-PRODUCTION, SELF IMPORT AND FREE CONSUMER)

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Keywords
Commercialization; Regulation; Natural Gas

Impact statement
The need for States to improve their regulatory framework in the natural gas market in a fast, simplified and isonomic way, in order to provide adequate conditions for supply by self-producers and self-importers, as well as the purchase and sale of the input in a market not regulated by consumers. free.

Highlights
Adoption of reforms and structuring measures in the provision of piped gas distribution services by the States, in order to reflect good regulatory practices, as determined by the National Energy Policy Council (CNPE), in Resolution 16 of June 24, 2019, which established energy policy guidelines and improvements aimed at promoting free competition in the natural gas market.

Abstract
The states have competence in relation to the natural gas distribution activity in Brazil, as provided for in article 25, paragraph 2, of the Federal Constitution, and may exercise the activity directly or delegate it to private companies, through the concession grant. Therefore, it is up to the States to create transition conditions for a competitive natural gas market effectively, considering the guidelines presented by CNPE, in RES16 / 2019, especially in relation to the characterization of free consumers, self-producers and self-importers and definitions on the need for early warning for free market migration and the existence of a minimum deadline for consumer return to the captive market. And, considering the federal government's prediction of the great social and economic impact to the country resulting from the opening of the natural gas market, it is mandatory that all measures be thoroughly studied and detailed by all entities. In this context, state regulatory agencies, which do not yet exist in some states, play an important role in effectively separating network marketing and service provision activities. It is up to them to act autonomously, with governance, transparency and a clear decision-making rite. Finally, the importance of minimal organization between states is noted, as the absence of any uniformity between local regulations could make the challenge of developing the natural gas market, especially the unregulated one, continue to exist. For example, adherence to tax adjustments by states, discussed in the scope of the National Council of Finance Policy - CONFAZ, is necessary to open the natural gas market, avoiding a fiscal war between the entities

Poster session **# S.09**

Carbon Capture and Storage and jurisdiction distribution in Brazilian institutional framework

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Keywords
CCS, institutional assessment, competences.

Impact statement
The growing demand for GHG emission mitigation solutions, globally, has promoted the expansion of research to enable CCS technology industrial scale projects. For the Brazilian case, the following challenges must be addressed: the acquiescence of a specific legal framework, namely the definition of jurisdiction and the behavior of the related institutions and agents.

Highlights
'- The jurisdiction distribution can impact CCS business - The more developed the institutional framework is, less risks tend to be input into CCS activities - There is no specific institution to regulate CCS activities in Brasil.

Abstract
The distribution of responsibilities, benefits and cost allocation along production chains has been a complex function in societies seeking commitment to climate change policies. They embed exogenous variables in the decision making of agents who, even though they are GHG emitters, produce goods that are important to society and that provide significant welfare gains. However, the distribution of gains and losses has been neglected in the formulation of public policies. It is about assigning legal competences and tailoring institutions for the development of CCS projects so that they are not negligent with essential factors for their intended purpose and, on the other hand, do not render them unfeasible due to the insertion of exogenous risks to the activity. In Brazil, we can point out two inaugural challenges to be faced and overcome, namely: the lack of legal framework involved as to its importance for reducing the country's carbon dioxide emission levels, especially in the definition of risks and responsibilities in the activities of storage in geological structure, and the lack of studies on the behavior of institutions and the agents. On related topics, ongoing research indicates that members of the Federal Government understand the importance of complying with the Paris Agreement, which is for the greater good, and that this may affect their own activity, but who would be responsible for coordination? How to make? It is not clear. Therefore, normative and institutional frameworks and stakeholders perceptions should be explored through the following question: what would be the institution with jurisdiction to authorize and regulate CCS activity in Brazil? We believe that, in short term, the distribution of jurisdiction will tend to be assessed in each project, given the nature of the core activity, and to be distributed between the environmental licensing authority and the sectoral regulatory agent. In the long run, the most efficient arrangement should seek to rationalize the number of participants so that decision-making about CCS activity can be less discretionary and more technically objective.

Poster session **# S.10**

Methodology for the construction of a low cost, high flux solar simulator for the production of synthesis gas through steam reforming of natural gas.

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Keywords
Natural gas steam reform, Solar energy, Solar simulator

Impact statement
Natural gas reforming is an important technology pathway for hydrogen production or synthesis gas. Using concentrated solar energy as a source for activating thermochemical reactions allows the most sustainable use of natural gas due to the reduction of greenhouse gases.

Highlights
* A sustainable methodology for stocking solar energy. *comparative evaluation of different reflective materials for the construction of paraboloid surface reflectors * Characterization of the different components of a high flux low cost solar simulator. * Relationship between chemical balance and blackbody reactor cavity temperature

Abstract
Hydrogen production through thermochemical cycles is an old research methodology that has been developed more strongly recently, in response to the worldwide demand for reliable and sustainable technologies that facilitate energy production. On the other hand, the study and development of innovative and affordable technologies that allow the use of solar energy as a useful energy source has become a research target around the world. This project seeks to harness the energetic power of hydrogen for power generation using solar energy as a heat source. Thus, the objective of this work is to describe the methodology of construction of a low cost high flux solar simulator to be used as a source of energy in the activation of thermochemical reactions of steam reform of natural gas. The methodology was divided into three main stages, the construction and characterization of the high flux solar simulator, the reactor cavity design and the thermochemical analysis of the natural gas steam reforming process. Two techniques for the characterization of the lamps used in the solar simulator were evaluated allowing to calculate the amount of useful thermal energy leaving the apparatus. Different materials for the construction of paraboloid reflectors were evaluated determining the concentration capacity and its losses. An initial project for the construction of the reactor cavity was proposed. By simulating the chemical equilibrium of the main equations of the reforming process, it was possible to relate the required working temperature within the reactor cavity to the temperature required for the thermochemical reactions to occur and to maximize the highest amount of synthesis gas production

Poster session **# S.11**

Numerical modelling of supersonic separator for biogas applications

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Keywords
Supersonic, Biogas, Biomethane

Impact statement
This paper reports the development of a model to study the behaviour of a supersonic separator device. The proposed model is one dimensional compressible flow solver with different equations of state. Therefore, the main impact of this paper is the development of a quick and flexible model that is suitable for simulations with different equations of state and different fluids.

Highlights
We elaborated a one-dimensional model of compressible flow with complex equation of state for monocomponent flow. The model is quick and uses complex equations of state. We are able to evaluate the flow of different fluids under various conditions and through diverse nozzle geometries. The developed model gives a starting point for a more complex model like 3D CFD analysis.

Abstract
The sugarcane industry has the challenge of becoming more sustainable. One of the main residues of the industry is the vinasse, which is originated from the ethanol production. An alternative use of the vinasse is the production of biogas, a mixture of methane and carbon dioxide. Even the biogas having great content of methane it has its applications limited because of the high content of carbon dioxide. In this context, a supersonic separator device to upgrade the biogas to biomethane may be an interesting solution. The main objective of this project is to create a model of a supersonic separator device to upgrade biogas to biomethane. This model should be fast, accurate and flexible enough to simulate different flow parameters and boundary conditions, and different compositions of the mixture. To model the supersonic separator device we built a first-order one-dimensional compressible flow solver using the Roe scheme in the Spyder, a Python code builder platform, using the thermodynamics properties library Coolprop. Therefore, we are able to have good precision on determining the state of the mixture in flow conditions. As a first step in the development of the model we are dealing with the monocomponent flow of carbon dioxide. Even it is not being representative of the objective case of this work, we use this flow as our first step flow because it is simpler to deal with the calculations of thermodynamics properties of monocomponent and yet we can verify almost all the phenomena of the mixture flow, as nucleation of condensate. We have tested the model under high-pressure conditions (8 MPa of total pressure in the inlet) and temperatures near the ambient temperature (320 K in the nozzle inlet) and deal with normal shock. In the simulations we calculate also the nucleation rate of condensate. The model was able to simulate compressible flow with shock waves and can calculate flow properties that is not implemented in commercial CFD codes, like nucleation rate of condensate. The code is very flexible and fast, but as a first order solver it has some numerical diffusivity that can be the source of inaccuracies in the results. However, the problem of inaccuracy can be reduced by increasing the refinement of the mesh of the simulations.

Poster session **# S.12**

Adjoint Optimisation in a Supersonic Swirling Separator

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Keywords
parametric optimization, adjoint method, supersonic swirling separator

Impact statement
This innovative optimisation of a supersonic swirling separator (including swirler and nozzle) uses 2D and 3D Euler equations, and the adjoint method to improve its performance, but keeping the same footprint. The method can be extended to turbine rotor/stator and rocket nozzles as well, either using Euler or Navier-Stokes equations.

Highlights
1. Succinct description of a supersonic swirling separator 2. Advantages of a supersonic swirling separator 3. Simulation of flow and adjoint solvers with optimisation results 4. The gains of parametric optimisation

Abstract
Supersonic separators of carbon dioxide are a relatively new technology which address two key factors in the Natural Gas processing: Firstly, it allows efficient separation of mixtures with large concentrations of carbon dioxide; and secondly, due to its compact size, it can fit in the reduced space available on the Floating Production Storage and Offloading (FPSOs) units. This project objective is to optimize the overall performance of the supersonic separator, allowing more room to the phase change processes that take place within its body, by delaying the position of shock waves. Owing to their strong dependence on both the occurrence of shock waves and the system geometry, this class of applications could greatly benefit from parametric optimization techniques. That is precisely the rationale behind the choice of the adjoint method, which can, in principle, serve both purposes. In that regard, it should be added that, although the physics of supersonic processes has received significant attention in the literature, there are few references that consider their optimization. The supersonic separator here studied, has two main components, a static swirl generator, which is responsible for the swirling flow, and a convergent-divergent nozzle, where the phase change processes take place. A shaft which sustains the swirler goes across the entire length of the separator. The working fluid is methane (CH4) with ideal gas behavior. For this simulation purpose, the open software Stanford University Unstructured (SU2) has been selected, which brings global visibility of University of São Paulo (USP) contribution in this arena, and allows other communities to benefit from the innovation provided by this project. A first contribution of this project collaboration in the SU2 community will appear in the next release of the code, concerning Discrete Adjoint and nozzle flows.

Poster session **# S.13**

ROTOR PERFORMANCE OPTIMIZATION OF A CENTRIFUGAL COMPRESSOR OPERATING WITH CO2 NEAR THE CRITICAL POINT

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Keywords
MEANLINE METHOD, CENTRIFUGAL COMPRESSOR, SUPERCRITICAL CARBON DIOXIDE

Impact statement
The need to transport and storage carbon dioxide with smaller turbomachinery makes centrifugal compressors the best choice, hence, these centrifugal compressors need to be optimized to maximum performance. The meanline method developed in this work provides a fast and precise first approach on the sizing of the centrifugal compressor rotor geometry.

Highlights
'- Centrifugal compressor rotor performance improvement - Meanline method coupled to NSGA-II - Fast and accurate method for preliminary results - Carbon dioxide operating near the critical point

Abstract
Due to its low capital cost, high efficiency with a simple layout and compact turbomachinery, Supercritical CO2 (S-CO2) power cycles have been arisen as an advantageous technology. Sandia National Laboratory is one the best researchers on S-CO2 providing reliable experimental data. The present work deals with a computer code implemented in MATLAB® by using mean line method to predict the rotor performance of a centrifugal compressor at design point and then perform an optimization routine using Non-dominated Sorting Genetic Algorithm genetic (NSGA-II) for maximization of the rotor isentropic efficiency. S-CO2 is considered as working fluid and the real-gas Span and Wagner equations of state have been used to calculate the thermodynamic properties of the fluid. Besides the maximum isentropic efficiency, the present work proposes some changes on the micro compressor developed by Sandia, considering only the rotor, which never reached the design point experimentally. With this changes the authors expect the compressor to achieve its design point. The results from optimization procedure are compared to available data of the Sandia compressor and the main results are discussed.

Poster session **# S.14**

CFD Simulation of a Radial Compressor Operating with Supercritical CO2

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Keywords

Supercritical CO2, CFD, Radial Compressor

Impact statement

Supercritical CO2 compressors are used at many stages of the CO2 value chain. Computer simulation can reduce compressor development costs by reducing the number of experimental tests. The performance gains of these compressors, achieved through optimization, are very important in this industry, with substantial savings by minimizing power consumption and compressor weight.

Highlights

CDF study to evaluate a radial compressor operating with supercritical CO2 was conducted. An improved equation of state for S-CO2 was used for the simulations. The 3D compressible turbulent flow simulation results presented good agreement with experimental data. Various aspects of fluid flow and thermodynamic behavior were investigated and elucidated.

Abstract

Computational Fluid Dynamics (CFD) has been widely used as a tool for designing, evaluating and improving turbomachinery, including compressors, turbines and pumps. Supercritical CO2 (SCO2) has been receiving wide attention due to its application in Rankine Organic Cycles (ROC) and Carbon Capture and Storage (CCS) systems. This project proposes to conduct a CFD study to evaluate a radial compressor operating with CO2 in the thermodynamic region above the critical point. Carbon dioxide allows its compression to occur above the critical point at suitable temperatures and high pressure. The compression work is therefore small, if compared, for example, to air compression. To obtain accurate results in terms of predicted efficiency and compressor performance, fundamental aspects of flows that evolve at supercritical condition should be investigated. The proof-of-concept supercritical CO2 micro-compressor developed at Sandia National Laboratories was selected to be the baseline model, which operates very close to CO2 critical point. The compressible turbulent flow in the impeller was simulated in 3D using the ANSYS® Turbosystem Package, which includes BladeGen® for the turbomachinery geometry, TurboGrid® for the mesh generation and CFX® for the simulation. A modified equation of state, based on NIST REFPROP database, was used to evaluate the thermodynamics properties of supercritical CO2. The impact of grid refinement on a given function was accessed by Grid Convergence Index (GCI) method. From the GCI analysis, it is clear that the numerical model was able to predict the different outputs for the three boundary conditions, so the numerical model can be considered reliable and accurate. Various aspects of the complex three-dimensional flow and the variations of the thermodynamic properties inside the impeller passage were investigated and elucidated.

Poster session **# S.15**

LNG in Brazil: Considerations of the Regulatory Context of Market Opening Designed by the New Gas Market

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Keywords
LNG terminals, PL 6.407 / 2013, New Gas Market

Impact statement
The Gas market in Brazil is changing fast, along with the new guidelines proposed by the federal Government in the recent iniciative named the "New Gas Market". The expected market opening has to be aligned with the harmonization of state and federal regulations. In the meantime, several projects involving the construction of new LNG terminals, many of them private, are in study.

Highlights
The expectation of raising the volume of imported LNG; Third party access to natural gas transportation routes and LNG terminals; The sale of shares held directly or indirectly in the transmission and distribution companies by the National Oil Company (NOC); The existence of several projects of LNG recovery terminals on the Brazilian coast, many of them conceived as private facilities.

Abstract
The Natural Gas transport activity in Brazil is a natural monopoly and, although third party access to transport pipelines is provided by the Petroleum Law (Law No. 9478/97), and by the Gas Law (Law No. 11.909 / 2009), the second law excludes LNG terminals from the provision of access. For some time now, players have been discussing a substitute sector of the Gas Law (PL 6.407 / 2013). At the Chamber of Deputies Commission on Mines and Energy, an application was presented in April 2019 to discuss the Bill. At a Public Hearing on May 22, 2019, there was a consensus of several entities present on some points, including: market opening; a harmonization of state and federal regulations; a harmonization of the gas industry with the electricity sector, which consumes half of the gas traded in the country; the adoption of the inbound and outbound transportation tariff model and access to gas flow routes to third parties, who would pay for the use. On June 24, 2019, the National Energy Policy Council (CNPE) issued Resolution 16, with energy policy guidelines aimed at promoting free competition in the natural gas market - the New Gas Market. According to its guidelines, It must be established as a matter of interest to the National Energy Policy that the agent occupying a dominant position in the natural gas sector promotes the total sale of the shares held directly or indirectly in the transmission and distribution companies. Resolution 16 was issued shortly after Petrobras sold the Associated Gas Transporter S.A. (TAG). At the same time, there are several projects of LNG recovery terminals on the Brazilian coast. In addition to Barra dos Coqueiros (SE) and Porto do Açu (RJ), a technical note released in August 2019 by the Energy Research Company (EPE), list 18 projects in four Brazilian regions. This paper aims to delineate the context of the regulatory scenario for the LNG market in Brazil, given that, in recent energy auctions, most successful thermal projects are natural gas thermoelectric plants linked to natural LNG terminals.

Poster session **# S.16**

Content analysis of workshops promoted by the Brazilian Natural Gas Law Centre, RCGILex, and their role to achieve the purpose of an Energy Law Centre

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Keywords
Natural Gas Law (11.909 / 2009); Energy Law Centre; Content Analysis

Impact statement
RCGILex provides information service by organizing the Brazilian Natural Gas law in a comprehensive perspective. The opinion of experts is important to promote and enrich discussions about gas market regulation and Energy Transition. Hence, the content analysis is fundamental to evaluate this contribution and to guide the next activities, including the expand to an Energy Law Centre.

Highlights
RCGILex is a Law Centre that provides free digital content and face to face workshops with specialists discussing the gas legal framework in Brazil. Energy transition needs to be build according to national rules and that reiterate the importance of the Law Centre to instigate a solid debate. RCGILex desires to reach other energy areas in order to collaborate the understanding to Energy Transition

Abstract
RCGILex is a law Centre that discuss gas market regulation in Brazil formed by a digital platform with website and interactive tool at the same time that workshops with specialists are often promoted. This three kind of activities addresses the gas market regulation in Brazil, updates and classical cases. The project to create and implement the platform started and in 2016 and until now 21 workshops were held with different specialists invited by the RCGILex team. This paper aims to analyses the content of the workshops from May 2018 till August 2019, totalizing 10 events directly connected with gas regulation. The study takes into account the fundamental phases of content analysis: pre-analysis, material exploration and treatment of results - inference and interpretation. This work presents the results of this analysis and point out the principal aspects and cases of gas regulation in Brazil that were discussed during the workshops. Also this study is important to guide the next activities to better cover the aims of the Law Centre and the desired intention to expand to an Energy Law Centre including the energy transition discussion.

Poster session **# S.17**

Study case: Best practice guidance for GHC management in the oil and gas sector

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Keywords
OGCI, Methane Emissions, MRV

Impact statement
The energy sector is the second source of Anthropogenic methane emissions; Oil and Natural gas will be part of the energy system for decades to come; There is uncertainty about the level of methane emissions from oil and gas operations; Oil and gas companies are making progress in quantifying and mitigating emissions;

Highlights
Almost 50% of the methane emissions can be reduced with no net costs; Quantification of methane emissions is difficult; The Paris Agreement "Rulebook" calls for scale up of national MRV effort; Regulatory standards, economic instruments and agreements between the industry and national authorities can all be part of effective and cost-efficient policies to address oil and gas methane emissions;

Abstract
This study provides a review of the UNECE guidance for developing and implementing effective monitoring, reporting and verification (MRV) practices, as well as for mitigating methane emissions, from the oil and gas sector. Methane emissions from this sector present a safety risk, are a waste of valuable energy resources, and are also a precursor of tropospheric ozone and a significant driver of climate change. In its discussion of MRV and mitigation opportunities, the UNECE document is intentionally "principles-based", recognizing that conditions vary greatly across oil and gas facilities, and that legal, political and institutional aspects differ by jurisdictions. It is important to notice that the UNECE document covers many aspects of methane management, along two dimensions: i. Physical dimension: All of the oil and gas supply systems are included, from exploration, extraction, gathering and processing, to long distance transmission and transportation, and finally refining and distribution to end users, and covering natural and technical circumstances that diverge greatly. ii. Institutional dimension: Methane management practices are addressed at the company, national and international levels, as well as discussions on how coordination and collaboration at the different levels can help enhance methane emission reduction. It´ shown that there are numerous initiatives, including regulatory efforts, public-private partnerships and industry collaborations, focusing on tracking and reducing methane emissions from the oil and gas sector. This study presents some of these initiatives and, in some cases, draws heavily on the technical guidance documents they have developed to inform the discussion of best practices for methane MRV and mitigation. The UNECE documents shall be faced as a useful complementary information document when considering MRV and mitigation plans.

Poster session **# S.18**

A real gas quasi - 1D model for the performance evaluation of supersonic separators.

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Keywords
CO2 Abatement, Supersonic Separators, Real gas, compressible Flow

Impact statement
One of the several challenges of the oil and natural gas offshore extraction in pre-salt reserves in Brazil, is the high content of carbon dioxide inside the wells, reaching values close to 80% in a molar fraction. This issue has a big impact on the crude extraction, due to the necessity of further expensive equipment occupying considerable deck space in platforms.

Highlights
Real gas model for compressible flow. Evaluation of condensation waves in supersonic flow Effect of oblique shock-waves in real gas flow. Performance of supersonic separators in function of the inlet conditions.

Abstract
Carbon dioxide is an important effluent for several processes, such as biogas production or natural gas extraction, for these processes, there is a necessity of finding new technologies to allow an economical and sustainable extraction of CO2. The supersonic separation concept fulfils all these requirements due to the absence of moving parts and simple operation, because its working principle is based on the strong temperature drop of gas mixtures at supersonic expansion as it occurs in supersonic channels. Eventually, at the right operating conditions, the mixture starts to nucleate and, therefore, it will drive the phase change. Nevertheless, the physical phenomena involved in this device is complex, because it involves phase change at supersonic speeds, which comprise compressible, multispecies, and multiphase and real gas flow. This work analysed these phenomena from a quasi-one-dimensional point view considering the following phenomena: supersonic flow, homogeneous nucleation, condensation waves and oblique shockwaves inside the device. Finally, was developed a real gas model for the preliminary estimation of the applicability of a supersonic separator for carbon dioxide binary mixtures, considering the device response on changes on the stagnation conditions (Pressure, temperature and concentration) at the separator inlet and their effects on the carbon dioxide separation and pressure recovery efficiency.

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