FUELING A CLEAN ENERGY FUTURE

2nd edition 2020

ACKNOWLEDGEMENTS

The University of Calgary would like to thank those who contributed to this publication:

Edward McCauley, PhD, FRSC
President and Vice-Chancellor

Ian Gates, PhD
Director, Global Research Initiative in Sustainable Low Carbon Unconventional Resources
Professor, Chemical and Petroleum Engineering

Jessica Tink
GRI Manager, Energy Research Strategy

Alejandra Bermudez
GRI Research Project Specialist, Mexico Initiative

Srijani Deb
GRI Institutional Research Facilitator

Melanie McDonald
Marketing and Communications Specialist, Office of the Vice-President (Research)

The University of Calgary's Creative Studio

Riley Brandt
Photography Specialist, University of Calgary Strategic Communications

Fritz Tolentino
Fritzology Photography

Erwan Nicholson

Trisha Loehr
TrishaJennReads

To all of the **University of Calgary researchers** who have contributed to this publication – thank you for your continued dedication and commitment to research excellence. The impact of your work is laying the foundation for a clean energy future that will benefit the environment, industry, and generations to come.

The University of Calgary would also like to acknowledge our partner, the **Southern Alberta Institute of Technology (SAIT)**, as well as all of our collaborators and supporting organizations that contribute to our research outcomes.

FOREWORD

In 2016, the University of Calgary, in partnership with SAIT, was awarded $75 million from the Canada First Research Excellence Fund (CFREF), and we launched our Global Research Initiative in Sustainable Low Carbon Unconventional Resources (GRI). We set our sights on tackling the greatest challenges associated with a low-carbon energy future, building on the efforts of our thought leaders across campus who were already engaged in high-impact energy research.

We are a little over halfway through this initiative, and a lot has changed for our institution, our province, the economy, and societies around the globe. No one could have predicted the circumstances we face today. A global pandemic, record low oil prices, rising unemployment rates, decimated corporations that have long been the backbone of our country.

However, throughout the hardships, there is no institution better equipped to rise to the challenge of these times than the University of Calgary. Teams from across campus have quickly mobilized to provide support to our communities, and our experts have been working with all levels of government to inform policy.

We will also be here to support the recovery of the oil and gas industry, work that is well underway. In Alberta, the oil and gas industry has long been the lifeblood of our province. But post-secondary institutions have been the heartbeat. The work conducted in our labs and classrooms shape the minds and outcomes of our future. UCalgary is delivering more impact now than ever before, particularly when industry and investors are looking towards less risk and higher environmental, social and governance standards.

Over the last four years, GRI researchers have made significant advances in green technology and reduced the carbon footprint of resource development. More than 300 researchers are engaged in three broad themes of research: heavy oil and bitumen, tight oil and gas, CO_2 conversion, and a cross-cutting technology assessment platform. We are working together with government and industry partners to translate our energy research into real-world solutions that will help us meet emissions targets, diversify our natural resources sector, and create jobs, thus growing the economy.

This publication is a testament to the hard work and dedication of an extraordinary team of multidisciplinary researchers working to create an innovative, green future. The Canadian oil and gas industry is ready for a resurgence, and the University of Calgary's GRI researchers are poised to make that a reality.

Edward McCauley, PhD, FRSC
President and Vice-Chancellor

In 2016, the University of Calgary, with the Southern Alberta Institute of Technology (SAIT) as partner, was awarded $75 million from the Canada First Research Excellence Fund (CFREF) to create the Global Research Initiative (GRI) in Sustainable Low Carbon Unconventional Resources (GRI). GRI was the first CFREF program in Canada to have a partnership between a University and a Polytechnic Institute.

It is now 2020 and GRI has created a vibrant ecosystem of energy research that spans multiple faculties, departments, community, and industry and government partners. Our three themes: 1. Heavy Oil and Bitumen, 2. Tight Oil and Gas, and 3. Carbon Dioxide Conversion, with cross-cutting platforms of technology assessment and data science, have engaged over 100 PIs and over 450 graduates students, postdoctoral scholars and research associates at the University of Calgary. The researchers in GRI are creating new solutions for some of the greatest global energy challenges.

We are now at the halfway point of GRI program and we have demonstrated that collectively, we can build new collaborations and work together in new and exciting ways. The partnership with SAIT is especially important given their strengths in prototyping — this has enabled many of our laboratory-based devices to be tested at larger scale bridging the gap between lab and field. Our research outcomes, both scholarly and applied, are making GRI a major hub for energy research in unconventional resources as well as low carbon energy.

The lifeblood of GRI is the passion and dedication of our incredible highly qualified personnel (HQP) — the graduate students and post-doctoral scholars. They are responsible for the many discoveries and novel solutions that are emerging from GRI and this book is an anthology to recognize and record their tremendous efforts.

This book lists active projects, current HQP, graduated and past HQP, research outcomes and spin-off companies that are emerging from GRI. This work demonstrates the success of GRI and the University of Calgary as a global leader in high impact energy research.

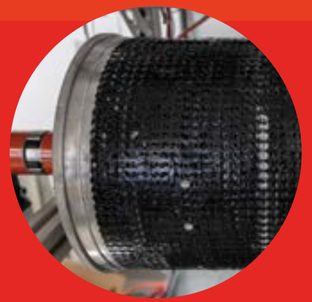
I find myself amazed by all the activities of our HQP and PIs and their ingenuity, resourcefulness and dedication and am excited by what will be accomplished in the second half of GRI program. I am very proud of our achievements and believe that you will enjoy this book as much as I have.

Excelsior!

Ian Gates, PhD
Director, Global Research Initiative in Sustainable Low Carbon Unconventional Resources
Professor, Chemical and Petroleum Engineering
University of Calgary

"This work demonstrates the success of GRI and the University of Calgary as a global leader in high impact energy research".

CONTENTS



THEME 1: HEAVY OIL & BITUMEN

Unconventional petroleum resources such as heavy oil or bitumen reservoirs are typically defined by being of low mobility due to the high viscosity of the oil – in these systems the oil can have viscosities in the thousands to hundreds of thousands to millions of centipoise. Thus, to enable production from these reservoirs, there are two requirements of a technically successful process – first, make the oil mobile (lower its viscosity), and second, move the mobile oil to a production well. The most used agent for mobilizing the oil is heat – in most recovery processes, steam is injected into the reservoir to heat the oil which makes it mobile enough for production. The key challenge we face is that to generate steam, fuel is combusted with consequent emission of greenhouse gas to the atmosphere. This also leads to the high cost for oil extraction in these recovery processes given the cost of the fuel required for steam generation. The heavy oil and oil sands industry must find new solutions for oil extraction that are low cost, low emissions, and energetically positive.

Theme 1 is focused on conducting research on how to make heavy oil and oil sands recovery processes more efficient with respect to energy intensity, emissions intensity, and cost. The research has multiple projects on the fundamentals of bitumen and the origins of its viscosity, improved steam-based recovery processes, low-emission recovery processes, as well as the use of additives (e.g., solvents and nanoparticles) with relatively low heating. Other projects include research on emulsions, bitumen structure and rheology, the fundamentals of multiphase flow in porous media, the fundamentals of nanoparticle interactions in bitumen-water systems, technology development and innovation of oil sands recovery processes, and steam generation.

Prof. Ian Gates leads Theme 1 and the Research Associate is Jingyi (Jacky) Wang. Other University of Calgary faculty members involved in the projects under Theme 1 are Profs. Getachew Assefa, Jalel Azaiez, Anne Benneker, Joule Bergerson, Sean McCoy, Hector De la Hoz Siegler, Michelle DoIgos, Hossein Hejazi, Jinguang Hu, Stephen Hubbard, Kristopher Innanen, Md Golam Kibria, Steve Larter, Qingye (Gemma) Lu, Brij Maini, Giovanniantonio Natale, Roman Shor, Samira Siahrostami, Bob Skinner, and Jennifer Winter.

BEYOND STEAM — ADDITIVES TO SIGNIFICANTLY IMPROVE THE EMISSIONS AND ENERGY INTENSITIES OF OIL SANDS RECOVERY PROCESSES

Ian Gates, Hossein Hejazi, Jalel Azaiez, Brij Maini, Steve Larter, Giovanni Natale, Qingye (Gemma) Lu, Hector De la Hoz Siegler

Background

At present, steam-based recovery processes for oil sands reservoirs are both energy and greenhouse gas (GHG) emissions intensive relative to other petroleum production processes. The key reason for the use of steam is that it is an excellent carrier of sensible and latent heat which raises the temperature of bitumen leading to a reduction of its viscosity, typically four orders of magnitude or more, so that it can be drained under the action of gravity. Solvent addition to steam has demonstrated that steam and solvent together is more efficient than steam alone. However, solvent-aided processes require large volumes of solvent and the reduction of energy and emissions intensity is small (after energy and emissions equivalent of solvent losses are considered) although oil rates are enhanced. The focus here is on the combined use of additives and warm water.

Research strategy

Here, the research steps away from solvents to examine additives that reduce bitumen viscosity or reduce interfacial tension (IFT) in the forms of surfactants (added or generated in situ), thin-film spreading agents, deasphalting agents, emulsion breakers, phase separation promoters and wettability alteration agents, at moderate temperatures (less than 100 C and saturated liquid water, has less than one-third of the energy of saturated vapor steam at steam-assisted gravity drainage (SAGD) conditions). The research has focused on experimental approaches for design and evaluation of additives with focus on functionalized nano and micro-particles and how they behave at interfaces. Furthermore, research on modelling the behavior of nano and micro-particles at interfaces has been examined.

Desired outcomes

The research will generate a rigorous understanding of the fundamental physics of these additives in oil sands systems. It is anticipated that the outcomes of the proposed research will lead to new oil sands recovery processes where most of the injected energy (and GHG emissions) is eliminated. Processes will be developed in which, at most, hot water is used with additives — since the latent heat is not injected, the energy content of the injectants are about two-thirds less than that of steam (vapor) based processes such as SAGD.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

The CO_2-steam-bitumen system, subsurface modeling and CO_2-steam recovery process design

Samaneh Ashoori
PhD student

Introduction

The intent of Samaneh Ashoori's research project is to design a new less-emissive process for heavy oil recovery. The novel concept of using direct contact steam generators (DCSGs) in the steam-assisted gravity drainage (SAGD) process is investigated through subsurface modelling of multiphase fluid flow coupled with geochemical reactions. The mechanisms of bitumen production enhancement due to the presence of CO_2 and CO_2 storage dynamics within the reservoir remains unclear. Mineral dissolution/ precipitations as a result of supercritical CO_2 injection in sandstones containing bitumen, along with aquathermolysis reactions are studied.

The research will provide directions for the design of DCSG-based SAGD recovery processes where the CO_2 emission intensity is reduced.

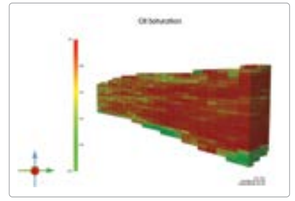


Figure 1

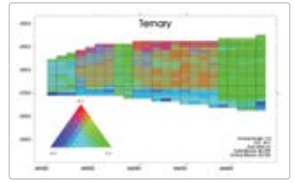


Figure 2

Results

Physical and chemical mechanisms involved in hybrid CO_2-SAGD processes for the recovery of heavy oil and bitumen are very complex. The complexity of modelling such processes originates from steam-oil reactions that generate CO_2 and H_2S, CO_2 phase behaviour at high temperature, gas-oil interactions, gas diffusion, dispersion and dissolution behaviour, and other rock-fluid and fluid-fluid interaction parameters. This study attempts to provide insights about effects of carbon dioxide injection on the gaseous products, in particular H_2S, of the aquathermolysis reactions in a SAGD operation through numerical simulation. The results indicate that CO_2 co-injection significantly reduces H_2S generation via aquathermolysis with enhancement of natural gas production from the reservoir. The mechanisms involved are investigated. The ultimate environmental benefits potentially outweigh lower revenue due to the lower bitumen production rate over the whole life of the process.

Final remarks

- Samaneh is currently working on the development of phase behaviour pressure-volume-temperature (PVT) modelling of the Athabasca oil sands, formation water and CO_2, as well as modelling of CO_2-water-rock interactions in Athabasca formation, identifying CO_2 trapping mechanisms in Athabasca oil sands and creating a three-dimensional SAGD reservoir simulation with minerals and aquathermolysis reactions.
- In the future, Samaneh will work on coupling geochemical batch reactions to oil reservoir simulation tools.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Dynamics of Janus colloids at interface

Mohammad Tanvir Hossain
PhD student

Introduction

This project aims to understand the behaviour of Janus colloids at interface through simulations and experiments. The main challenge of this project is to understand the physical phenomenon that causes the movement of a single particle or a collection of particles that sits on the interface. At the single particle level, the particle movement is affected by Brownian motion and surface force because of the different chemistries present on the particle surface. The project will investigate the effect of size, shape and chemistry at the surface and combination of suspending fluids. These results will then be extended to a collection of Janus particles at the interface. Their behaviour is expected to be influenced by particle-particle hydrodynamic interactions. The outcome of this research will be significant for applications in enhanced oil recovery as a new technology to induce mobility of interfaces.

Results

Mohammad Tanvir Hossain started his research with translation and rotation of amphiphilic Janus spheres, then extended it to Janus rods at interface. He implements mesoscale methods to simulate motion of Janus particles at interface, depicted in Figure 1, and quantifies their diffusion, shown in Figure 2. One of the major challenges that the research team overcame was to quantify the effect of aspect ratio on the diffusion of Janus rods. The team has analyzed and established the effect of diffusion due to change in aspect ratio of Janus rods at interface, shown in Figure 3.

Final remarks

- The diffusion of nanorods increased with the decrease of the aspect ratio of Janus rods.

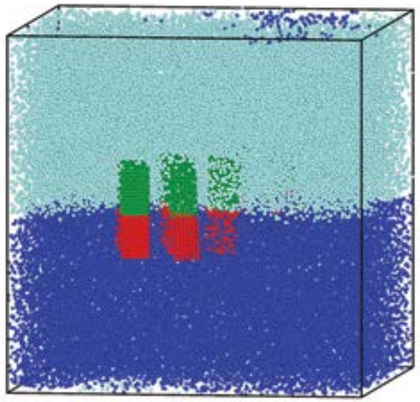


Figure 1

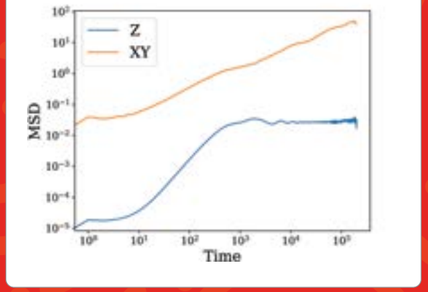


Figure 2

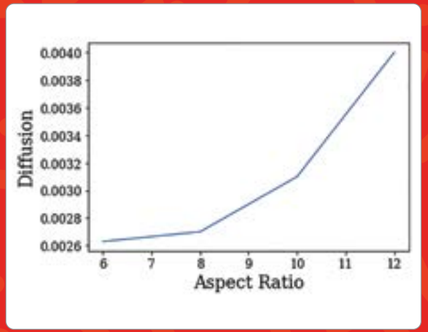


Figure 3

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Roughness and wettability

Xuemin Huang
PhD student

Introduction

This research is focused on the contact angle variety in the system of liquid-solid-air rough contact. Deionized (DI) water and rough surfaces with different wettability are used in experiments to find the relation between contact angle and surface roughness.

Results

Xuemin Huang has found that roughness enhances original wettability, i.e., it makes hydrophilic surfaces more hydrophilic or hydrophobic surfaces more hydrophobic. Also, the distribution of the contact angle on the periphery of the water droplet has a similar distribution trend (close to normal distribution) with that of roughness (valley depth) on the contact area, shown in Figures 1 and 2. Curvature of the solid contact area increases the contact angle as well as roughness. Hence, curved solid surface can increase or decrease original wettability depending on its hydrophilicity or hydrophobicity. Additionally, Xuemin has created a model of contact angle on rough surface in terms of roughness, surface curvature, contact length and liquid volume.

Final remarks

- The distribution of contact angle on contact periphery can be linked to distribution of roughness.
- On curved cylindrical rough surfaces, the contact angle is affected by curvature. On hydrophobic surfaces, the curvature increases contact angle. But in the presence of roughness on hydrophilic surfaces, curvature can decrease or increase the contact angle depending on the roughness and curvature level.

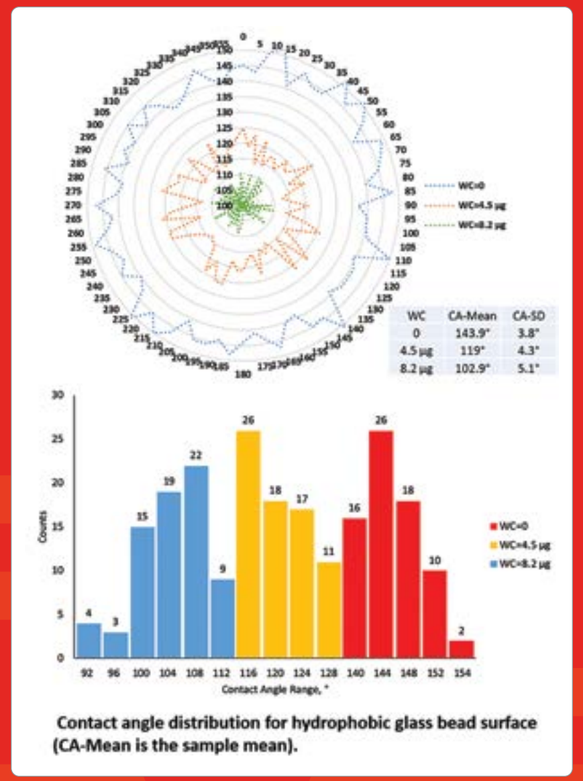


Figure 1

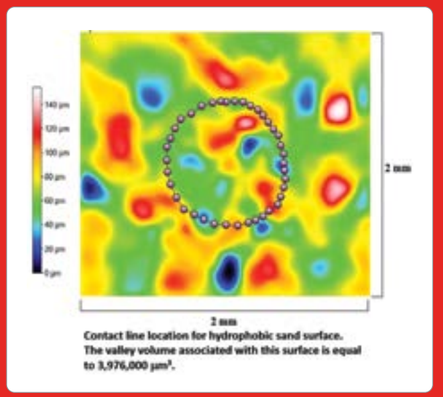


Figure 2

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Ranjani Kannaiyan
Research Associate

Introduction

Bitumen consists of surface-active species. The related surface tension and surface charges determine the efficiency of bitumen extraction from oil sands. The aim of this study is to relate the effect of temperature, addition of aliphatic solvents and addition of surfactants to the surface-active behaviour of asphaltenes in bitumen. The findings of this work would provide a deeper insight into the role of asphaltene in reducing the surface tension, which will enable modification of processes for enhanced oil recovery and handling of bitumen emulsions.

Results

Asphaltenes behave as a separate colloidal solid phase distributed in the maltene phase at low temperatures, up to approximately 60 C. Further increase in temperature causes the asphaltene rich molten colloidal phase to coalesce into the liquid maltene phase. Addition of anionic surfactant lowered the surface tension of bitumen by 6 per cent up to 65 C. The combined effect of the additives has been shown to decrease the surface tension of bitumen by 23 per cent at up to 50 C, beyond which the rate of decrease in surface tension is low.

Final remarks

- The mechanism by which n-alkanes reduce the surface tension of bitumen is solely by dispersive forces whereas anionic surfactants cause the same effect by acid-base interaction with asphaltenes.
- Temperature plays a dominant role in controlling the surface tension of bitumen.
- Sodium dodecyl sulfate (SDS) acts as a dispersant and releases the maltenes occluded between the asphaltenes molecules.
- The optimum choice of temperature and n-alkane/surfactant concentration for low surface tension depends on the asphaltene concentration/composition in bitumen.

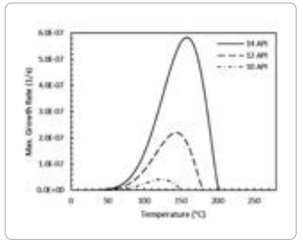
Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Instability of parallel flow of two immiscible liquids in a pore

Young Hoon Lee
PhD student

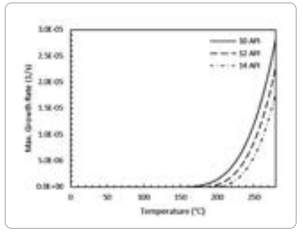
Introduction

The effectiveness of steam-based oil sands recovery processes is controlled by heat transfer from steam (latent heat) to bitumen within the reservoir — the greater the heat transfer, the lower the oil phase viscosity, and consequently, the larger the drainage rate. Furthermore, in the two-phase zone of steam condensate and bitumen, if an oil-in-water emulsion forms, the drainage could be enhanced due to low viscosity of the water host phase. The research conducted here is on the instability at the interface between two parallel flows of steam condensate and bitumen through a uniform planar pore using linear stability analysis. A characteristic equation has been derived to determine the growth rate of the instability as a function of the wavenumber. The results have been applied to the case of steam-assisted gravity drainage (SAGD).



Results

The results show that the instability is only possible when the top fluid is denser than the bottom fluid, and the instability is governed by a dimensionless group relating the ratio of the gravitational force to interfacial tension. The interfacial tension has a stabilizing effect resisting the destabilizing gravitational force, limiting the range of wavelengths of unstable disturbances to be longer than a minimum critical wavelength. For the SAGD process, the stability of the interface can change depending on the temperature because the bitumen density can be higher or lower than that of steam condensate depending on the temperature. The instability is possible only over a specific range of temperatures given the densities of the steam condensate and oil in the reservoir.



Final remarks

- A characteristic equation which determines the growth rate as a function of the wavenumber determined the conditions required for instability.
- There is a temperature for SAGD where the growth rate becomes maximum for the case of steam condensate above and bitumen below and a minimum temperature where instability occurs for the case of bitumen above and steam condensate below.
- The results suggest that there might be an optimal temperature where in situ oil-in-water emulsions form with consequent enhanced drainage rates.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Shruti Mendiratta
Postdoctoral Fellow

Introduction

Emulsification is an efficient method to aid the hydraulic transport of viscous heavy oils as the oil-in-water emulsions exhibit significantly less viscosity compared to the parent oil. Dr. Shruti Mendiratta, PhD, aims to achieve stimuli responsive emulsions for viscous oil mobilization and easy transportation. Her goal is to develop specialized nanoparticles that respond to a variety of external triggers and to investigate the stabilization/destabilization of their corresponding Pickering emulsions.

Results

Shruti has synthesized functionalized Fe_2O_3@HaP (HaP = Hydroxyapatite) nanoparticles and their corresponding Pickering emulsions. She has fabricated microfluidic models to study the stability of mineral oil-water emulsions. This work is currently under review in Langmuir.

Figure 1a exemplifies that these HaP-based Pickering emulsions are magnetic and exhibit pH-responsive behaviour. Figure 1b shows that the size of emulsions decreases with an increase in pH. Emulsion stabilization as well as destabilization can be achieved for at least ten consecutive cycles on changing the pH followed by ultrasonication. The microfluidic studies have established emulsion stability and their flow without coalescence under shearing flows. She believes this is very beneficial for transportation of petroleum-based emulsions.

Shruti has also synthesized functionalized Fe_2O_3@β-calcium phosphate magnetic microsquares and has investigated their movement using a solenoid under different currents. Figure 1c shows that, interestingly, the particles align to form one-dimensional (1D) pillars under electromagnetic fields. The Pickering emulsions formed using these particles can also be destabilized using the solenoid.

Final remarks

She has concluded that the size of the emulsions prepared using Fe_2O_3@HaP nanoparticles are smaller when the pH is elevated.

- Microfluidic studies allow visualization of emulsions under flowing conditions and show that they are highly stable as the size variation at the beginning and at the end of the channel is negligible.
- The stability and amount of Pickering emulsions formed using Fe_2O_3@HaP nanoparticles are influenced by the viscosity of the oil phase. More efforts are required to study their efficacy on bitumen and heavy oil.
- The destabilization of Pickering emulsions formed using Fe_2O_3@β-calcium phosphate depends on the strength of the solenoid. Further study is required with solenoids with a strength greater than 0.1 Tesla.

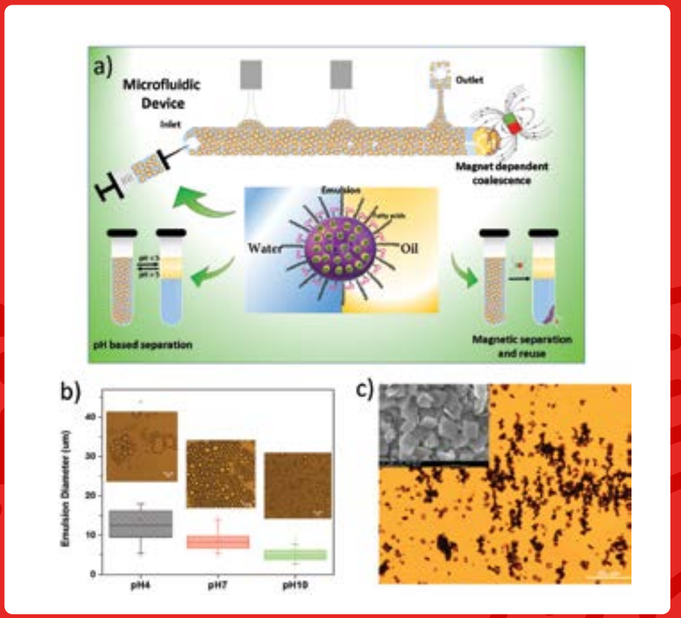


Figure 1

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Valorization of oilfield resources

Michael Mislan
PhD student

Introduction

Michael Mislan aims to develop novel methods for simultaneously remediating and valorizing oil field resources, including bitumen and oil sand tailings.

Results

Michael developed a method for biodegrading bitumen using common, over-the-counter digestive enzymes to release sugars and fatty acids from constituent fossilized soil organic matter. The results of this work were published in Scientific Reports — a research journal from the publishers of *Nature*. He has also optimized a method to inexpensively solidify oil sand tailings into a form that is amenable for kiln firing into ceramics by returning the clays to a feldspathic form.

Final remarks

- Michael's work suggests that principles from the earth sciences literature can be applied to the remediation and valorization of bituminous reservoir components which are natural terminal products of the biogeochemical carbon cycle.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Enhancing heavy oil recovery using rich solvent-steam assisted gravity drainage (RS-SAGD) method

Vijitha Mohan
Postdoctoral Fellow

Introduction

The research of Dr. Vijitha Mohan, PhD, examines approaches to overcome the difficulty in extracting highly viscous heavy crude or bitumen by introducing higher percentages of solvents (more than 60 per cent) along with steam in a steam-assisted gravity drainage (SAGD) well configuration. Usage of solvents along with steam reduces steam requirements leading to decreased steam-to-oil ratio (SOR) and energy-to-oil ratio, making the recovery process more economical with less greenhouse gas emissions — that is, cleaner and lower-cost bitumen extraction.

Results

Initial work involving literature reviews shows that increasing solvent percentage to 20-30 per cent in steam increases the oil recovery rate. Solvents like hexane and diluent are found to be efficient solvents compared to that of lower and higher hydrocarbon solvents. Injecting 20 per cent of solvents with steam has increased the oil recovery rate to 80-90 per cent. SOR is found to decrease by 50-60 per cent, and the energy-to-oil ratio is found to decrease by 20-60 per cent when injecting solvents along with steam. Modifying injection strategies of solvent and steam have also contributed to increased oil production with reductions in solvent losses. Vijitha's research targets to further increase the solvent percentage to 60 per cent in steam and study its impact on the oil recovery rate. The key economic concern is the lost solvent to the reservoir — the research will examine methods to maximize the recovery of solvent from the reservoir.

Final remarks

- Vijitha's planned research involves simulating rich solvent-SAGD operations (RS-SAGD) using diluent as a solvent (hexane will be used as a surrogate).
- The impact of the variation of solvent injection along with injection pressure will be studied. Solvent will be either injected simultaneously with steam or alternatively, steam along with solvent can be injected.
- The results will be compared with SAGD as well as other existing steam-solvent recovery processes including expanding solvent-SAGD (ES-SAGD), solvent assisted-SAGD (SA-SAGD) and solvent-aided process (SAP).

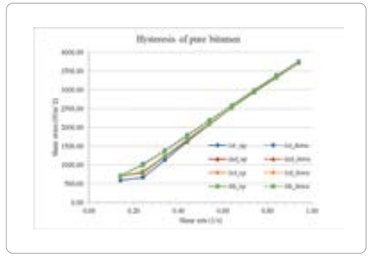
Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Viscosity behavior and hysteresis of bitumen and solvent/bitumen mixtures

In Young Park
MSc student

Introduction

The understanding of the rheological properties of bitumen is essential in oil production and transportation, in that the wrong prediction and measurement of flow can lead to inaccurate results. However, a full understanding of the rheological properties of pure bitumen and mixtures of solvent/bitumen remains unknown due to its complex behaviour. In this experiment, the viscosity of pure bitumen and binary mixtures of solvent and bitumen (heptanol/bitumen and heptane/bitumen) were measured versus the shear rate over several cycles of increasing and decreasing the shear rate to investigate the rheological behaviour of bitumen and bitumen/solvent mixtures.



Results

In Young Park and the research team observed both shear thinning and shear thickening behaviour depending on the direction of the shear rate change. That is, hysteresis of the viscosity was observed over multiple cycles of increasing and decreasing the shear rate. Based on extensive research, the team postulates that the hysteretic behaviour results from the structural changes of the bitumen and solvent-bitumen mixtures. They tried to link these observations to the microstructure of bitumen, and that colloidal particles of asphaltenes influence the formation of the internal network and that this can be broken down and built up with increasing and decreasing the shear rate.

Final remarks

- The non-Newtonian behaviour and hysteresis of the pure bitumen and the binary mixtures of bitumen/solvent (heptane and heptanol) is explained with the microstructure of bitumen and bitumen/solvent mixtures.
- The effect of the concentrations of solvent on the viscosity of bitumen is investigated.
- This research of bitumen and bitumen/solvent mixtures provides insight into understanding the complex rheological behaviour of bitumen.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Md Mohosin Rana
PhD student

Introduction

Greenhouse gas (GHG) emissions from oil and gas production rose up to 23 per cent from 2000 to 2017. But climate change and growing energy demand require drastic reduction in the GHG emissions. Additives (e.g., catalysts and solvent) delivery could be an option to improve energy efficiency of crude oil recovery by mitigating GHG emissions and making the process more environmentally friendly. The principal objective of this project is to develop a thermoresponsive polymer-based nano-/microcarrier system for the delivery of these additives to the reservoir. This smart-carrier system will enable the use of state-of-the-art additives to increase the ultimate resource recovery while reducing energy intensity and recovery expenses.

Results

Initially, Md Mohosin Rana investigated the polarity effect of synthesis-solvents on the microstructural, mechanical and thermoresponsive properties of the Poly(N-isopropylacrylamide) (PNIPAm) hydrogels. The synthesis-solvent polarity does not compromise the thermoresponsive behaviour of PNIPAm hydrogels, but Figure 1 depicts how it can effectively modulate their microstructure and mechanical properties. Mohosin's study revealed that synthesis-solvent polarity could be an option to regulate the thermomechanical properties of the hydrogels to work in harsh reservoir environments. His next step is to develop interpenetrating network (IPN) hydrogels of PNIPAm and cellulose nanofibrils (CNF) to make it more economically viable and environmentally friendly. He believes that such a small-scale encapsulation device will transform enhanced oil recovery operations.

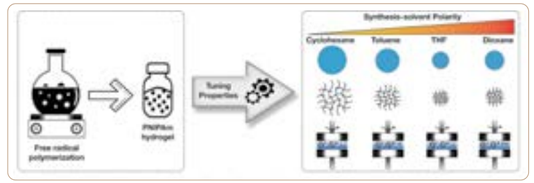


Figure 1

Final remarks

- The synthesis-solvents of different polarity indexes can be used to regulate thermomechanical properties and porosity of the PNIPAm hydrogels.
- Selection of synthesis-solvents can be an additional design variable in addition to crosslinking density and copolymerization to control the characteristics of the hydrogels.
- In the future, developing PNIPAm and CNF-based IPN hydrogels would be a better choice in terms of strong mechanical performance.
- Small-scale polymer hydrogel-based smart-carrier should be an attractive additive delivery option for more economically viable and environment-friendly crude oil recovery applications.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Cellulose-based materials applied in wastewater purification

Yuxuan Ren
PhD student

Introduction

Yuxuan Ren aims to design and synthesize cellulose-based composites to be applied in water purification, including the removal of heavy metal ions, dyes or oils. Her current project is to combine metal-organic frameworks (MOFs) with cellulose as a form of porous aerogels to achieve a better removal performance. She anticipates that her project will provide an alternative application of cellulose to wastewater purification.

Results

Yuxuan has successfully fabricated the cellulose aerogels as the base material and is trying to combine it with MOFs. She expects this composite could achieve good removal performance towards different pollutants. This composite is expected to exhibit great physical properties.

Final remarks

- Cellulose aerogels have been successfully synthesized. The next step is to combine with MOFs and start the removal testing with different pollutants.
- She expects this composite could possess great physical properties and achieve good removal performance towards different pollutants.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Computational modelling of heat transfer and particle tracking in a steam generator

Mohan Sivagnanam
PhD student

Introduction

The objective of this project is to understand heat transfer phenomenon and particulate transport in once through steam generators (OTSGs) using computational fluid dynamics (CFD). In situ oil sands recovery processes for bitumen extraction rely on steam, consuming natural gas to generate heat. This leads to carbon dioxide emissions which is the major cause of environmental impact from in situ steam-based oil sands recovery processes such as steam-assisted gravity drainage.

Results

The project involves a three-dimensional multiphase CFD modelling of a lab-scale OTSG unit, as well as a full field OTSG unit. Mohan Sivagnanam found that the main location of erosion in the heat transfer tubes within the OTSG occurs at the bends and is associated with the rotating flow through the bend. The simulations demonstrate phase change from liquid water to vapour water with the onset of multiphase multi-regime flow.

Final remarks

- The findings show that the wall temperature determines the evolution of multiphase behaviour in the steam generator.
- The CFD simulations results identify the phase distribution profile along the heat transfer tubes.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Heat transfer analysis of nanofluid forced convection into channels with extended surfaces

Rasa Soleimani
PhD student

Introduction

In this project, Rasa Soleimani thoroughly investigates the effects of the nanofluids on heat transfer of channels with extended surfaces from the hydrodynamic point of view. It has shown how the geometrical parameters are related to the hydrodynamics of the system. It has also shown how the nanoparticles can be effective in such systems to improve the heat transfer performance.

Results

In channels with extended surfaces, there are multiple parameters that can be investigated to specify their effects on heat transfer. One of the most important parameters is the height of the blocks mounted on the surface. This research has shown that increasing the height of the blocks can also have a negative effect on heat transfer. It has shown that there is a non-monotonic connection between increasing the height of these blocks and the average Nusselt number that describes the heat performance of the system. There is a critical height value that should be considered correctly. The non-monotonic behaviour has been explained by lots of hydrodynamic parameters such as the vorticity.

Final remarks

- Heat transfer has been analyzed using the Buongiorno's two-component model in a channel with extended surfaces.
- The nanoparticles concentration distribution affects the heat transfer enhancement.
- The height of the blocks affects the Nusselt number with a non-monotonic trend.
- The non-monotonic behaviour is related to the hydrodynamics of the system.
- The other geometrical parameters and the flow regime influence the heat transfer enhancement.

Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Electrokinetic and coagulation study of warm lime softening process

Lu (Josh) Zhang
MEng student

Introduction

Josh Zhang's research is to understand the interactions and electrokinetic properties of the two most common particles ($CaCO_3$ and $Mg(OH)_2$) in the steam-assisted gravity drainage (SAGD) warm lime softening (WLS) and to investigate the impact of water chemistry variations on the dose of a cationic polymer. Thermodynamic modelling was also used to predict precipitates. The charges of both particles varied depending on the water chemistry variable. Silica and humic acid were found to have a significant impact on the coagulant dose. The results of this study will be highly relevant to WLS on-site chemical dosage evaluation and operational controls, especially during a WLS effluent off-specification event.

Results

During the electrokinetics study, Josh found that the two most common particles ($CaCO_3$ and $Mg(OH)_2$) can present either positive and negative charges depending on the solution pH or presence of potential-determining ions. Humic acid, silica and clay also have a great impact on the surface charge of particles. Thermodynamic modelling was beneficial in determining and understanding the potential precipitates in each system. During the coagulation study, Josh found that humic acid and silica can significantly drive the coagulant dose. Carbonate and lime can also drive the coagulant dose but not as much as humic acid and silica. Metal ions, clay and MgO did not show much effect on the coagulant dose.

Final remarks

- For SAGD WLS operation, it is important to understand the surface charge of the water being treated as it can impact the selection and dose of a coagulant.
- Thermodynamic modelling can be used to predict the potential precipitates forming during the process to have a better understanding of the charge development.
- Zeta-potential (ZP) measurement can be a useful tool for coagulation process optimization and can provide insights beyond the traditional jar testing.

NEXT-GENERATION ADAPTIVE WELLS AND OPTIMAL PLACEMENT FOR IMPROVED RECOVERY

Roman Shor, Ian Gates, Stephen M. Hubbard, Steve Larter, Kristopher Innanen

Background

Well placement and completion design are often not optimized relative to reservoir geology and thus do not perform to their maximum possible ability. On average, steam conformance in steam-assisted gravity drainage (SAGD) well pairs is about 50-60 per cent of well utilization — that is, only 50-60 per cent of the well is effectively used for steam injection and oil production. This is due to a number of factors, including: an omission or poor understanding of the reservoir geology, poor placement of the well pair or ineffective injection or production strategies. All of these reduce the potential production of the well pair and lead to reduced revenue, higher steam use, lower efficiency and higher per-barrel emissions.

Research strategy

By enhancing imaging of the reservoir, through techniques like seismic-while-drilling (SWD), an improved structural model may be obtained. Further improvement may also be achieved through the development and deployment of high-resolution reservoir models for well planning and production optimization. This project seeks to develop improved workflows for seismic-while-drilling data acquisition and processing, evaluate new well designs outside the typical parallel-horizontal well pair paradigm and then develop and optimize control strategies for intelligent well completions. Well completions which include real-time sensing and distributed downhole static and dynamic inflow/outflow devices are being evaluated via simulation against a high-fidelity reservoir model, and in the future, in the field. Improved drill string dynamics modelling will enable feedforward and model predictive control, which will also better drilling performance. Finally, research typically reserved for unmanned aerial drones, including swarming and peer-to-peer communication, is being evaluated for autonomous drilling robots which may be used for improved, distributed sensing or improved production.

Desired outcomes

This project will present a new workflow to collect and analyze seismic-while-drilling data, develop and deploy new real-time drill string dynamics models suitable for real-time control, propose new well plans and wellbore completions for improved steam conformance, and develop a framework (and prototype) for autonomous downhole drilling robots. This project has already produced several invention disclosures and aspects of the research has been presented at international conferences and at industry workshops. Field trials for the use of drill string dynamics models has commenced in conjunction with an external project.

Next-generation adaptive wells and optimal placement for improved recovery

Impact of non condensable gases on FCD performance

Andres Betancur
MSc student

Introduction

The goal of Andres Betancur's research is to examine the use of different types of flow control devices (FCDs) combined with non-condensable gas co-injection to improve the performance of steam-assisted gravity drainage (SAGD). The non-condensable gas reduces the amount of steam injected into the process, thus yielding lower environmental impact. A vast amount of experimental data on FCD flow tests from industry is being analyzed in this project. A new model has been developed, which closely matches the experimental data. The model will be used to optimize the FCD design and the amount of non-condensable gas used.

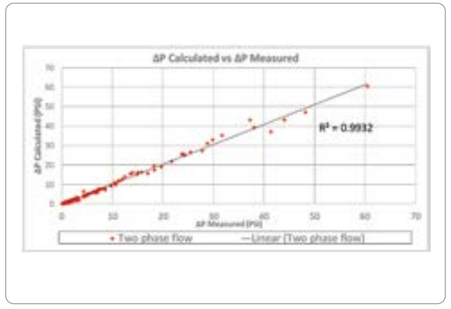


Figure 1

Results

Figure 1 shows 247 measured points for a six millimetre converging-diverging nozzle FCD. This experiment was for the flow of oil, water, steam, and nitrogen. With temperatures, pressures and qualities up to 270 C, 6340 kilopascals 9.8 per cent, and 100 per cent, respectively, the maximum steam flashing inside the FCD is 4.6 per cent. The model developed in this work provides an excellent match of the measured pressure drop. The model has been shown to match for another 2500 data points from 18 other experiments for three types of FCD: friction, hybrid design and converging-diverging nozzle. These results indicate that this model can be used for modelling this type of flow through restrictions.

Final remarks

- The results show the new model applies to different FCD architecture with excellent predictions of the pressure drop for multiphase flow.
- By using the model, an optimization of the FCD design will be conducted to yield the most uniform injection of steam-gas mixtures along injection wells and fluid production from production wells in SAGD operations.
- The model will be used to reduce the steam-to-oil ratio, thus improving process economics and environmental impact.

Next-generation adaptive wells and optimal placement for improved recovery

Reservoir characterization of channel-belt strata, McMurray Formation, northeastern Alberta

Jordan Curkan
MSc student

Introduction

Jordan Curkan aims to map the vertically stacked channel-belt strata of the McMurray Formation in northeastern Alberta. Heterogeneity of point bar deposits varies both laterally and vertically, so when stacked bars are considered, heterogeneity increases substantially. Historical performance indicators including production and steam-to-oil ratio as well as reservoir monitoring data such as four-dimensional (4D) seismic data and thermocouple data are used to show how geology affects project performance.

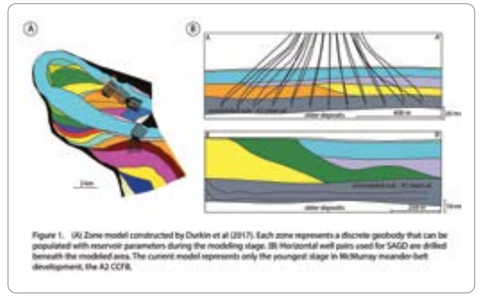


Figure 1. (A) Zone model constructed by Durkin et al (2017). Each zone represents a discrete geobody that can be populated with reservoir parameters during the modelling stage. (B) Horizontal well pairs used for SAGD are drilled beneath the modelled area. The current model represents only the youngest stage in McMurray meander-belt development, the A2 CCFB.

Figure 1

Results

Using several novel approaches, Jordan was able to apply a recently revised stratigraphic framework to map the deposits of the McMurray Formation within the study area. Her research team believes detailed characterization of these units is a crucial step in the reservoir delineation stage. She will aim to publish this work in the near future. The next step of the project includes expanding the geomodel created by Durkin et al and published in the Journal of Sedimentary Research in 2017 to include the newly mapped deposits underneath the previously seismically constrained unit (Figure 1).

Final remarks

- Jordan was able to map stacked channel-belt deposits in the study area within a recently revised stratigraphic framework.
- Net-to-gross mapping within each belt revealed significant lateral heterogeneities in sandstone content and reservoir quality over short distances.
- Heterogeneity of a reservoir becomes more complex when vertically stacked channels are considered.
- Heterogeneous boundaries between stacked belts can significantly impact production performance.

Next-generation adaptive wells and optimal placement for improved recovery

Robots and sensors for subsurface exploration and device emplacement

Juan Oziel De la Fuente Valadez
Postdoctoral Fellow

Introduction

Dr. Juan Oziel De la Fuente Valadez's research involves mechatronic design of devices aimed at improving state-of-the-art in data acquisition from oil sands. The objective is to develop autonomous devices and sensors that can be used to gather data from the oil sands deposits located in Alberta. His vision imagines a swarm of autonomous robots mobbing inside nonconsolidated media that can form a sensor network and get useful data from the deposits to increase the efficiency of the production process. So far, he has worked on the design and development of the propulsion mechanisms for the devices. A second project involves the design of a drill string emulator that can be used to test new soft sensors and control algorithms in the lab.

Results

Juan and his team designed a bioinspired peristaltic mechanism for the traction of the robots. The design was published at the 2020 International Conference on Robotics and Automation. The paper was titled "Single Actuator Peristaltic Robot for Subsurface Exploration and Device Emplacement". A simplified diagram of this mechanism is shown in Figure 1. The mechanism was tested for the first time on nonconsolidated media, it generates peristaltic motion using a cam/follower configuration.

Final remarks

- Juan has established a basic mechanism for the autonomous robots.
- The pressure in the deposits will limit the battery life to a few hours at a time.
- A sensor package for the robots is being designed.
- Juan and his team can now test control algorithms on the drill string emulator.

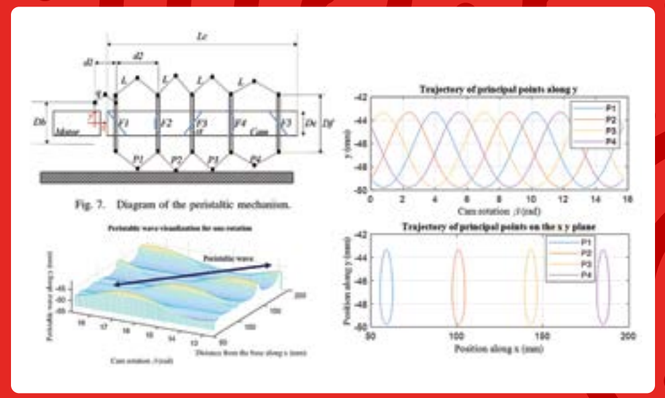


Figure 1

ASPHALTENE DEPOSITION KINETICS/STRUCTURE

Michelle Dolgos, Ian Gates, Samira Siahrostami

Background

A key component of heavy oil and bitumen that presents a major control on their viscosity is the asphaltene fraction of these oils. The asphaltenes also host most of the sulphur and metals within the oil that cause issues with respect to environmental impact and processing of the oil. Furthermore, the asphaltene fraction is a major source of naphthenic acids within the oil which can be corrosive causing major issues for processing of the oil. However, it is costly and difficult to separate asphaltene from heavy oil and bitumen — very little is understood on the structure and chemical nature of asphaltene. The separation of asphaltenes and deposition is not well understood in porous media.

Research strategy

In this subproject, the research team will understand the structure of asphaltenes, resins, and bitumen to provide insight into its properties and behavior as well as micromodel experiments to understand the deposition of asphaltenes in small pores. They aim to use local structural probes such as total scattering (pair distribution function method), small angle scattering, and/or Extended X-ray absorption fine structure (EXAFS) as well as rheological analysis to understand the structure of these materials. The structures can be investigated in a static state or as a function of temperature, pressure, time, etc.

Desired outcomes

The team will work with the computational group studying the molecular origin of heavy oil/bitumen viscosity to gain an atomic level understanding of the structure-property relationships of each system.

Asphaltene deposition kinetics/structure

Green chemical synthesis of piezoelectric thin films

Stuart Burns
Postdoctoral Fellow

Introduction

Through the conversion of electrical to mechanical energy and vice versa, piezoelectrics are key functional energy materials for next-generation sensors, actuators and ultrasonic devices. The current industry standards of piezoelectrics, however, are lead-based compositions. Given strict environmental policy over the past few decades, there is a recognized need for micro-electromechanical systems (MEMS) made from non-toxic elements and processes. To this end, Dr. Stuart Burns, PhD, aims to establish a new green method for synthesizing potassium sodium niobate ($K_{0.5}Na_{0.5}NbO_3$) thin films with properties that compete with current industry piezoelectrics.

Stuart is also working on the Asphaltene Deposition Kinetics/Structure project with the goal of establishing the molecular structure and kinetics of asphaltenes, known as “the cholesterol of petroleum”. These aromatic molecules drastically hinder the viscosity of heavy oil in pipelines and are not well understood. Through X-ray scattering, they aim to understand the aggregation of these molecules and explore the chemical alteration in order to modify solubility. This project is still in the early stage of development as it was greatly impacted by the global pandemic.

Results

Aqueous-solution chemistry has been established to form lead-free piezoelectric thin films with sound structural properties.

Final remarks

- Stuart’s next steps are to optimize the synthesis process to improve the film’s properties and further explore the strain and structural behaviour of these thin films.

Asphaltene deposition kinetics/structure

Oxide ion conduction mechanisms in bismuth perovskites

Alisa Paterson
Postdoctoral Fellow

Introduction

Dr. Alisa Paterson, PhD, aims to understand the mechanisms underpinning ionic conduction in bismuth perovskite materials such as sodium bismuth titanate. Using X-ray, neutron diffraction and total scattering as tools, she has been fitting data to determine the crystallographic structure of these materials as a function of temperature. This work will reveal the unique structural distortions and oxygen vacancies that enable the high oxygen conductivities in these bismuth perovskites and will help guide the development of materials for emerging energy applications, such as intermediate temperature solid oxide fuel cells.

Results

Alisa has collected X-ray diffraction and total scattering data from the Advanced Photon Source at the Argonne National Laboratory, and neutron diffraction and total scattering data from the Spallation Neutron Source at the Oak Ridge National Laboratory. Between sodium bismuth titanate samples with different doping and stoichiometry, the structural changes seem minimal, despite their differing ionic conductivity. However, these are preliminary observations. Further investigation is ongoing as data collection was only recently completed in July 2020.

Final remarks

- Alisa has observed the expected phase transitions from monoclinic to tetragonal to cubic with increasing temperature in the sodium bismuth titanate materials.
- Rietveld refinements of the X-ray diffraction data confirm these phase transitions.
- Her next steps include large-box modelling, which will allow her to fit the X-ray and neutron scattering data simultaneously to create a valid and meaningful model of the material, ultimately providing insight into the mechanism of ionic conduction.

Asphaltene deposition kinetics/structure

Structure and property relationships in lead-free piezoelectric solid solution (x)$NaNbO_3$ — (1-x)$BaZrO_3$

Tom Rowe
PhD student

Introduction

Piezoelectric materials are integral in the manufacturing of sensors, actuators, power sources, touchscreens and almost any electronic device that responds to touch. The most common piezoelectric on the market is lead zirconate titanate (PZT), but with increased knowledge of lead toxicity, a major thrust has been made into synthesizing and characterizing new lead-free alternatives. Thus, Tom Rowe has been working on completely explaining the structure and property relationships in lead-free piezoelectric materials.

Results

Tom has been using various solid-state synthesis techniques to make high-quality samples for both structure and property characterization. The end results show a complicated set of phase transitions throughout the solid solution resulting in a complex series of properties related to the composition. Using various characterization techniques such as polarization under electric field, dielectric permittivity and strain measurements, he saw a transition from a ferroelectric to relaxor material. These categories of materials each have different strengths and weaknesses depending on the application and will be evaluated for these various end uses.

Final remarks

- The solid solution displays a complicated structure evolution.
- Depending on composition, the material displays ferroelectric, relaxor or paraelectric properties.
- This material is being evaluated for a variety of applications.

Asphaltene deposition kinetics/structure

Structure-property relationships in group ii substituted bismuth pyrostannate ($AxBi_2$-$xSn_2O_{7-\delta}$)

Bryan Zanca
PhD student

Introduction

Bryan Zanca's project involves the search for new materials that can be utilized as solid electrolytes in solid oxide fuel cells (SOFCs). To date there are several issues that surround the most common solid electrolytes such as mismatched thermal expansions and chemical reactivity between device components. Therefore, new materials are needed to help lower the current operating temperature of SOFCs. Currently, Bryan is exploring materials that crystalize in the pyrochlore crystal class such as bismuth pyrostannate ($Bi_2Sn_2O_6O'$), which has been shown to be an oxide ion conductor.

Results

Several novel compositions have been successfully synthesized by doping alkaline earth cations into the $Bi_2Sn_2O_6O'$ structure (A_xBi_2-$xSn_2O_{7-\delta}$; A=Ca^{2+}, Sr^{2+}, Ba^{2+}). This introduces defects known as oxygen vacancies into the structure which have an effect on the observed properties. The structure of each material has been studied using high resolution synchrotron X-ray diffraction performed at the Advanced Photon Source at the Argonne National Laboratory. In addition, highly dense polycrystalline ceramics have been prepared for all compositions, which is essential for property measurements.

It is Bryan's hope that by investigating these materials for oxide ion conductivity it will lead to a better understanding of how this property manifests itself and how the structure can be manipulated to enhance the properties.

Final remarks

- Several novel compositions have been successfully synthesized by traditional solid-state methods.
- Each material has been studied using high resolution X-ray diffraction.
- Sintering conditions for each composition have been refined to produce dense ceramics.

MOLECULAR ORIGIN OF HEAVY OIL/BITUMEN VISCOSITY, ASPHALTENE SELF-ASSEMBLY

Samira Siahrostami, Ian Gates, Michelle Dolgos

Background

Asphaltenes are known to be the reason for the extreme viscosity of heavy oil/bitumen. Molecular level calculations targeting the behavior of asphaltenes, can be used to relate molecular structure and interactions to macroscale physical, chemical and mechanical properties. This project aims to use a combination of quantum mechanical calculations and molecular dynamics (MD) simulations to model the behavior of asphaltenes and bitumen. Quantum mechanical methods determine an approximate numerical solution to the Schrödinger equation and thus incorporate electronic effects of chemical interactions. On the other hand, classical force fields used in dynamics simulations can be applied to simulate how asphaltene and bitumen systems evolve over time.

Research strategy

The research will address the effect of chemical composition of oil, solvent, temperature, pressure and water-oil interaction on the structure and viscosity by choosing proper simulation models, at different thermodynamic conditions. Using MD simulations, it can provide molecular descriptions of self-assembly and the oil diffusion process.

Desired outcomes

The project will be able to derive the viscosities from MD simulations and make direct comparisons with experimental results. In addition, to study the asphaltene self-assembly, the asphaltene-asphaltene interactions and asphaltene-solvent interactions are investigated. The results provide a molecular level understanding on the origin of heavy oil/bitumen viscosity and the asphaltene self-assembly mechanism.

Molecular origin of heavy oil/ bitumen viscosity, asphaltene self-assembly

Nikhil Poolakkal Aravindakshan
Postdoctoral Fellow

Introduction

Asphaltenes are known to be the reason for the extreme viscosity of heavy oil/bitumen. Dr. Nikhil Poolakkal Aravindakshan, PhD, uses a combination of quantum mechanical calculations and molecular dynamics simulations to unravel the origin of asphaltene self-assembly and its relationship to observable physical phenomena. Asphaltene structure is obscure, and Nikhil uses a few possible structures based on the available knowledge on asphaltenes. He computes viscosity from the simulations which can directly be compared to experimental results. He analyzes the simulations using various tools for possible interactions in asphaltenes that result in self-assembly and thereby high viscosity.

Results

Simulations of pure asphaltenes and solvated asphaltenes have reproduced the viscosities in the right order of magnitude and showing the correct trend versus temperature. The solvated asphaltene simulation results have a direct comparison to experimental results from Western Canada asphaltenes, and Nikhil's results show reasonable agreement with them though he slightly overpredicts the viscosity values. Nikhil had to use a mix of four unique structures to come up with an asphaltene model. He calls it a 4A model.

Simulations were analyzed with the help of radial distribution functions. Aromatic C-C radial distribution functions show a peak at 5 angstrom (Å), which is an indication of pi–pi interactions between asphaltene molecules. This was more clearly observed in the pure asphaltene simulations than in the solvated case, because in the solvated asphaltene sample the solvent-asphaltene interactions replace some of the asphaltene-asphaltene interactions present in the pure sample. Hydrophobic pocket is another major form of interaction between asphaltene molecules, which is evidenced in Nikhil's aliphatic C-C radial distribution functions. Other possible interactions like hydrogen bonding, metal coordination and acid-base interactions appear to be very minor contributors to self-assembly of asphaltenes.

Final remarks

- Molecular dynamic simulations of asphaltenes made with their possible structures can reproduce their known viscosity values.
- Nikhil was able to successfully simulate a pure asphaltene sample by using four unique possible structures.
- Pi-pi stacking along with hydrophobic pockets appear to be the major contributors to asphaltene self-assembly.

GREEN SOLVENTS

Hector De la Hoz Siegler, Jinguang Hu, Hosein Hejazi

Background

Enhancing the environmental and economic feasibility of bitumen and heavy-oil recovery is key to ensure the market and social acceptance of the hydrocarbons locked in the Canadian oil sands. The project aims to develop a deasphalting and low energy solvent-based recovery process that uses safe, environmentally friendly and low-cost solvents. Using solvents instead of steam to drive the mobility of oil in the reservoir will translate in a major reduction in the footprint of the oil sands industry.

Using residual biomass (agricultural, forestry and industrial waste) as a feedstock for the production of solvent will provide a dual benefit: reducing the carbon intensity of the bitumen-recovery process and eliminating GHG emissions associated with current waste disposal technologies. Producing solvents from biomass, either through thermochemical or biochemical routes, is technically feasible. Common solvents obtained from biomass include lactates, levulinates, furfural and glycols. The solubility of bitumen and its fractions in most of these solvents have never been studied. However, as most of them have polar character it is expected that they might provide differential solubility for maltenes and asphaltenes fractions, hence serving to deasphalting the bitumen.

Research strategy

To accelerate the discovery and technology translation, this project has a three-prong research strategy, with each prong being pursued in parallel: (1) Solvent screening: measure the properties of different heavy/oil bitumen fractions in pure biomass-derived solvents and use performance metrics to select most desirable solvent. (2) Residual biomass deconstruction: the research explores biochemical, catalytic and/or thermochemical processes to efficiently convert different types of biomass into simpler building blocks that can serve to synthesize a green solvent. (3) Development and scale-up of the green solvent production process: work on fermentative and catalytic pathways for synthesizing green solvents starting from simpler building blocks present in deconstructed biomass is being done.

Desired outcomes

- The research aims to identify three to five different solvents that will be able to effectively mobilize bitumen and heavy oils at relatively mild temperatures.
- The goal is to demonstrate the process for converting residual biomass into one of these solvents at lab scale and to transfer the technology to one of GRI partner companies.

Green solvents

Green biomass-derived solvents: a biorefinery approach toward a green oil sand industry

Mohammad Alikarami
PhD student

Introduction

Mohammad Alikarami's research project will determine the most suitable biomass-derived green solvent to facilitate the recovery of bitumen from Alberta's oil sands resources and establish an optimized biochemical pathway to produce these green solvents from biomass at mild environmental conditions. Using biomass-derived solvents helps to reach the circular economy and metabolic engineering helps to reveal the underlying mechanism for the biochemical production of the solvents.

Results

After a comprehensive literature review, about 25 different solvents were chosen and procured to perform a rapid screening to quantify their suitability as a bitumen mobility enhancer. Interfacial tension, viscosity and solubility of bitumen in the solvents were used as deciding metrics. A spinning drop tensiometer apparatus was employed to characterize the interfacial tension and interaction forces between solvent and bitumen at varying temperatures and solvent ratios. Figure 1 shows early interfacial tension experiments on one of the selected solvents.

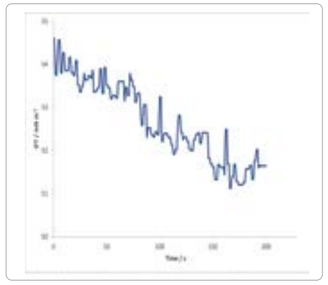


Figure 1

Mohammad and his colleagues designed a high pressure and high temperature reactor for acid hydrolysis to convert the lignocellulosic biomass to the mixed sugars, using fermentation to convert it to the desired solvents. Figure 2 shows the designed and ready to operate hydrolysis reactor.

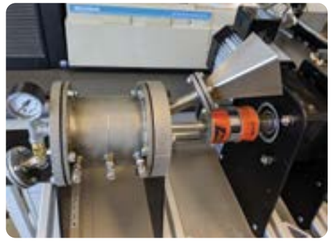


Figure 2

Final remarks

- Screened solvents change the interfacial properties of the bitumen-solvent mixture. Decreased interfacial tension may be beneficial for improved bitumen recovery.
- Viscosity measurements at 50 C showed lower viscosity for pure toluene compared to mixture of toluene/screened solvents. However, both pure and mixed solutions demonstrated a drastic decrease in the viscosity of bitumen. The experiments at other temperatures are in progress.

Green solvents

Converting biomass to lipid and green solvent

Shouyun Cheng
Research Associate

Introduction

Alberta is rich in agriculture and forest residues. The conversion of these biomass residues to valuable products such as lipids and solvents is beneficial. There are two objectives of this project. The first objective is to develop an efficient biochemical approach to convert biomass to lipid. This is a two-step process consisting of converting biomass to sugar using a *Ganoderma applanatum* culture and subsequent fermentation using a *Auxenochlorella protothecoides* culture. The second objective is to develop an effective biomass catalytic conversion method to produce hydroxymethylfurfural (HMF). The goal is to design, characterize and test novel metal-loaded HZSM-5 catalysts to maximize HMF selectivity and yield.

Results

Shouyun Cheng, PhD, obtained three biomass feedstocks (flax straw, wheat straw and sawdust) with particle size less than one millimetre using the mill machine. Additionally, he found that the glucose concentration of the biomass fermentation product solution is 0.01 per cent. This lower concentration may be due to the massive glucose accumulation in the cell walls of the *G. applanatum*. He found that the glucose content of the biomass hydrolysis using C-Tec 2 is 0.02 per cent without pre-treatment of the biomass feedstock. Shouyun has completed an article titled "Current Methods of Converting Biomass Into Glucose — A Critical Review" and he is currently working on a second article titled "Biomass Conversion to Hydroxymethylfurfural Using Different Catalysts".

Final remarks

- The glucose concentration of biomass fermentation product solution is not high, and further experiments such as using *G. applanatum* and algae together need to be conducted.
- The pre-treatment of biomass before hydrolysis is required to improve sugar yield.
- The prepared catalysts will be applied for converting biomass to HMF using a thermochemical catalytic approach.

Green solvents

Thermochemical and catalytic pathways at lab-scale to convert different biomass wastes

Jesus Fabricio Guayaquil-Sosa
Postdoctoral Fellow

Introduction

Dr. Jesus Fabricio Guayaquil-Sosa's research project focuses on converting biomass into green solvents and using them for bitumen extraction in wells. His goal is to design, build and operate a pyrolytic bench-scale reactor to transform biomass into value-added chemicals (e.g., green solvents).

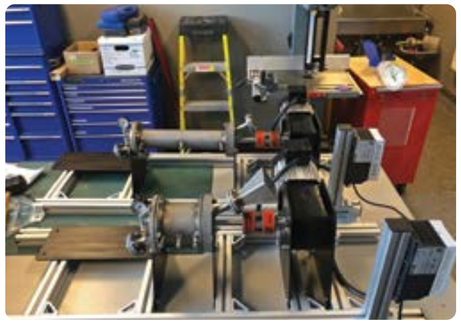


Figure 1

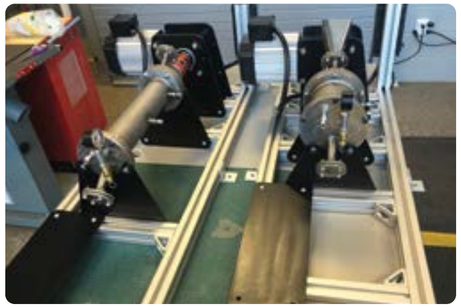


Figure 2

Results

Since the beginning of Jesus's appointment at the University of Calgary in Fall 2019, he has worked in conjunction with the Southern Alberta Institute of Technology (SAIT) to build the pyrolytic batch-scale reactor. Since then, two pyrolytic batch-scale reactors were built and delivered to the University of Calgary. Jesus has been working on the units to make them operational, and the first experimental results were retrieved in July 2020. Figures 1 and 2 show the pyrolytic bench-scale reactors for green solvents production from biomass.

Final remarks

- Jesus has found that using a rotary bench-scale pyrolytic reactor can convert biomass into green solvents (green chemicals).
- Jesus has concluded that the ouzo effect can be applied towards an enhanced extraction of bitumen from wells using a green solvent-oil emulsion.

Green solvents

Oil-in-water emulsions stabilized by cellulose filaments

Amir Varamesh
PhD student

Introduction

Pickering emulsions have applications in many different areas including oil recovery and the pharmaceutical and food industries. The use of green and sustainable particles represents an evolution in stabilizing the Pickering emulsions. Cellulose is a renewable, biodegradable, low-cost and abundant resource which has captured attention as a stabilizing agent of Pickering emulsions due to their amphiphilic characteristics. Amir Varamesh's research aims to investigate the potential of cellulose filaments (CFs) and their capability to stabilize oil-in-water emulsions. The emulsification mechanism of CFs, and the effect of ionic strength and pH on the stabilized emulsions are investigated in Amir's project.

Results

So far Amir has demonstrated that the CFs can efficiently stabilize oil-in-water emulsions. He showed that the formulated emulsions using CFs are more stable than emulsions stabilized by cellulose nanofibrils (CNFs), TEMPO-oxidized CNFs and cellulose nanocrystals (CNC). Results showed that the obtained emulsions are stable at a wide range of ionic strength. Also, the CF can stabilize emulsions under acidic and basic pH ranges.

Final remarks

- CFs can provide more stable oil-in-water emulsions in comparison to the other types of celluloses.
- The stabilized emulsions by CFs are salt-resistant and stable at a wide range of ionic strength.
- The prepared emulsions by CF are stable under acidic and basic pH ranges.

PHORETIC FLOWS AT PORE SCALE

Giovanniantonio Natale, Hossein Hejazi, Anne Benneker

Background

Low salinity water injection has been identified as an effective way to enhance oil recovery. In this context, it can be speculated that diffusiophoretic flow, which is established when there is a gradient in ions concentration, can act as an additional mechanism to vehiculate droplets or particles in small (dead-end) pores, not accessible by “simple” hydrodynamic flow.

The role played by diffusiophoresis in oil recovery and flow in porous media is still to be fully established. The project intends to quantify this effect through controlled experiments in dead-end pores via microfluidics. More in details, an important issue in studying complex fluids in porous media is to reproduce the petrographic geometry and the surface forces of real rocks within lab-scale experiments. Microfluidics can reproduce with high fidelity geometrical details of the structure of real porous media.

To enhance diffusiophoretic flows in dead-end channels, active particles able to generate gradients on their surfaces could be also employed to generate microflows and micro-mixing. Engineered micro-particles could provide a solution to enhance chemical gradients and can be activated specifically where it is needed. Chemo-hydrodynamic coupling between this solution and external salt gradients and the effect of confinement will be investigated.

Research strategy

To explore the role and magnitude of diffusiophoresis in oil recovery, the research employs a combined approach between microfluidic, confocal and fluorescence microscopy, and micro-PIV. Various salt and pH gradients will be generated in dead-end microfluidic channel geometries. The magnitude of the velocity and flow streamlines in the case of multiphase systems (oil droplets in water) will be explored. The effect of confinement of the oil droplets in the channels will also be considered.

The effect of pH responsive active colloids designed and fabricated in Dr. Natale’s Laboratory (patent filed) will be employed to generate microflows as potential solution to enhance oil mobilization in dead end channels.

Desired outcomes

This research will create a visualization and quantification of the flow fields generated by diffusiophoretic flow by salt or pH gradients in presence of oil droplets. Additionally, determination of the effect of confinement (ratio between oil droplet radius and channel characteristic size) on the efficiency of the process is expected. Finally, this research will quantify the impact on the velocity profile and efficiency of the oil recovery process in presence of active particles.

Phoretic flows at pore scale

Emulsion transport through porous media driven by temperature gradients

Di Pu
MSc student

Introduction

Di Pu’s goal is to investigate the thermophoretic behaviour of oil-in-water emulsion droplets by means of microscopic images of droplet movement and comparing the experimental results with those calculated by theoretical models to modify the theoretical descriptions of thermophoresis. Di will also seek possible applications of thermophoresis in enhanced oil recovery processes.

Results

Using a statistical physics approach, Di has modified a three-parameter model for thermophoretic behaviour of colloidal particles suspended in deionized water. The application of this model in oil-in-water emulsion droplet needs to be verified with the experimental studies.

Final remarks

- The magnitude of the Soret coefficient depends on the number of binding sites which may scale linearly with the surface area of the colloidal particle.
- The sign change of the Soret coefficient is related to the binding energy between solvent molecules and the functional groups on colloidal particles and the chemical potential of water molecules at local thermodynamic equilibrium conditions.

Phoretic flows at pore scale

Water treatment using electrokinetic phenomena

Mansoureh Rashidi
PhD student

Introduction

Mansoureh Rashidi is studying electrokinetic phenomena such as electrophoresis in water treatment to separate oil-in-water emulsions. In this research, she uses amphoteric surfactants to charge the droplets and drive them under the influence of an external electric field. These types of surfactants containing both anionic and cationic hydrophilic groups can change the charges of the droplets at different pH levels. As the direction of motion in electrophoresis is a result of the charge of the droplet, amphoteric surfactants result in a change in direction of the electrophoretic movement when pH is changed. This significantly increases the flexibility and controllability of the separation process.

Results

Mansoureh has done the literature review on electrophoresis of the droplets. She has also designed her experiments. In this research, she will study the effects of amphoteric surfactants on the electrophoresis of emulsions by measuring different parameters such as the surface potential and electrokinetic velocity of the droplets at different conditions including different droplet size, electric field, pH and ionic concentration. She conducts her experiments in simple microchannel geometries, in which she has a high control of local field strength and environmental properties such as pH, where she visualizes the electrophoretic transport of emulsions stabilized by amphoteric surfactants. After this, the effect of temperature gradient on electrophoresis of emulsions will be investigated alongside the aforementioned parameters.

Phoretic flows at pore scale

Investigation of shock electrodialysis and electrokinetic instabilities on the microscale

Milad Rezaei
MSc student

Introduction

Milad Rezaei is designing a microfluidic chip for the investigation of ion transport in porous media. By applying an external electric field over an ion-selective membrane in contact with a salt solution, ions will selectively be removed from the solution, creating depletion zones. In shock electrodialysis (shock ED), in the presence of a surface charged porous media the ion concentration polarization (ICP) phenomenon can be used to desalinate water using deionization shocks. Shock ED is a promising, energy-efficient technology for water treatment applications.

Results

By applying electric current over an ion-selective membrane in contact with a fluid containing charged species, three distinctly different regions can be observed in the current-voltage diagram: the ohmic, limiting and over-limiting regimes. In the ohmic regime, the relation between current and voltage follows Ohm's law and is approximately linear. In the limiting regime, the current will not increase with increasing voltage, as a result of transport limitations at the membrane interface. In the over-limiting regime, current again increases non-linearly when increasing the voltage. Shock electrodialysis occurs in this over-limiting current regime, where large depletion zones exist at the membrane interface. The cause of over-limiting current in such a system is an intricate electrokinetic phenomenon. Different parameters can impact the electrokinetic phenomenon such as pH and ionic strength of the inlet solution, and flow rate. In this research, Milad will visualize this process to gain a full understanding of the physical phenomena.

Final remarks

- Electric field intensity has a direct impact on shock electrodialysis and electrokinetic visualization.
- The pore size of the porous medium directly impacts on the shock electrodialysis phenomenon.
- Surface charge of porous materials can affect the shock electrodialysis and electrokinetic instability formation.

Phoretic flows at pore scale

Flow and heat transfer in micro-systems

Mohammad Zargartalebi
Postdoctoral Fellow

Introduction

Mohammad Zargartalebi, PhD, analyzes fluid flow and heat transfer in complex microscale geometries. His focus is on the mechanistic understanding of heat transfer at small/large scales. He is trying to find simple ways to make large improvements in energy transfer. Optimizing heat transfer and fluid flow is his main goal in this project.

Results

Mohammad has made excellent contributions to energy industry enhancement. He has published several papers on heat removal from microchips. In his recent publication in *Physics of Fluids*, he has shown that small modifications of porous media at pore-level can significantly enhance hydrodynamic and heat transfer behaviours. He has meticulously explained the underlying mechanisms, using particulate flow analysis, and accordingly designed a system that improves both heat removal and friction, which is the first of its kind in the energy field.

Final remarks

- Mohammad has shown that small changes in the microscale porous medium can have large impacts on fluid flow and heat transfer.
- He has found that simultaneous heat transfer improvement and friction reduction is possible if the system is designed based on the governing mechanisms.
- His research also reveals that practical porous media, whose structure is heterogeneous can, depending on flow conditions, outperform or underperform the homogeneous system.

MASS TRANSPORT AND EDGE CHAMBER EFFECTS

Anne Benneker, Ian Gates, Giovanniantonio Natale

Background

Transport at interfaces, boundaries and through pores can significantly limit the overall efficiency of a variety of processes such as oil recovery, catalytic processing and water treatment. Interfacial instabilities such as viscous fingering further reduce overall process efficiency. Larger process yields are achieved if mass transport throughout porous media is increased and instabilities can be controlled. Understanding, manipulation and control of this mass transfer is required to optimize the efficiency of current and future recovery processes.

Research strategy

This project is investigating a variety of strategies for the enhancement of mass transfer throughout porous media and at system boundaries. Finding innovative ways to increase the transport of viscous fluids through smart use of external and internal stimuli will enhance the overall efficiency of processes including enhanced oil recovery. Currently the use of local temperature, concentration and potential gradients is investigated through a combination of experimental and numerical investigations. Utilization of low-grade waste heat, geothermal energy and naturally occurring gradients in temperature and concentration will allow for synergetic increases of transport with minimal environmental impact. The research is focused on transport involving visco-elastic fluids such as polymer solutions through confined spaces and at interfaces.

Desired outcomes

This project seeks to develop and test strategies for mass transport enhancement that require minimal energy and material investments. These technologies should be applicable in existing and novel processes. The team aims for fundamental understanding of the transport mechanisms to be translated to real-world implementation through collaborative research and extensive modeling of scale-up possibilities.

Mass transport and edge chamber effects

The use of electric field to control viscous fingering in porous media

Benedicta Nwani
PhD student

Introduction

Benedicta Nwani is currently investigating the possibility of reducing viscous fingering in porous media by inducing electroosmotic flow in the fluids using an externally-applied electric field. Her goal is to investigate the physics involved in the process and the subsequent changes that occur at the fluid-fluid interface under varying conditions such as brine ionic composition, valence, varying viscosity ratio, varying surface charge and wettability. This investigation is conducted numerically using a finite element software (COMSOL Multiphysics) and experimentally using a Hele-Shaw cell.

Results

Benedicta has modelled viscous fingering in a two-dimensional rectilinear system with fluids of different viscosity ratios. The results show that the viscosity ratio between the displacing and displaced fluid affect the number of fingers as well as the fingering pattern formed in the system. Additionally, she has modelled electroosmotic and pressure driven flow in a single electrolyte. The next step in modelling is to combine the two models to see the effect of electroosmotic flow on the fingering.

An experimental setup has been designed for the observation of electroosmotic effects on viscous fingering. The rectangular Hele-Shaw cell will have in situ electrodes for the application of an electric field. Visualization of the viscous fingering will be done for a variety of field strengths and other experimental conditions to be able to fully understand the effect of electroosmotic flows on interfacial instabilities encountered in porous media.

Final remarks

- The use of electric fields to control viscous fingering is a promising avenue to control transport in porous media.
- Experimental evidence in combination with numerical modelling will lead to an increased understanding of the observed phenomena.
- These results are relevant to oil recovery systems, and have applications in water treatment and environmental remediation.

Mass transport and edge chamber effects

Three-dimensional stability of interfaces at the chamber edge

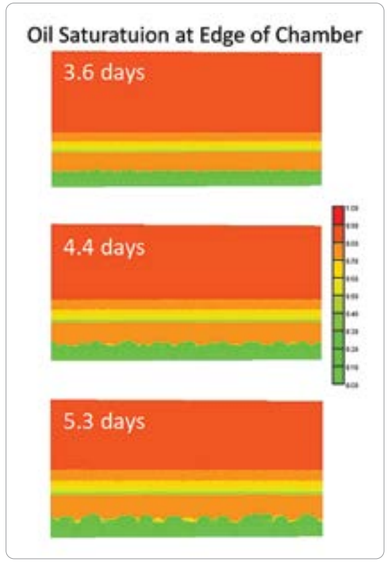
Qian Zhou
MSc student

Introduction

In this project, Qian Zhou analyzes the instability of the steam chamber interface by using numerical simulation in a three-dimensional (3D) model with superfine grid focusing on just the steam chamber edge. The model describes the evolution of small-scale perturbations at the steam-oil interface and the interaction of the thermal and gas fingers. The focus of this study is to gain understanding of dynamic behaviour of steam fingering in the steam-based recovery process by examining the physics (e.g., the interaction between heat transfer, liquid drainage, gas buoyance and phase behaviour) and analyzing the dimensionless forces distribution (e.g., capillary number, Bond number, Lewis number) at the chamber edge.

Results

Since thermal efficiency is a key issue in steam-based oil recovery, the main outcome of this research is to understand how the instability occurring at the chamber edge contributes to heat transfer and its capability to enhance heat transfer there. A 3D ultrarefined thermal model has been developed. The results reveal that instability at the chamber edge can affect the conformance of steam chamber and thus influence thermal efficiency. In addition, instability of the steam-oil interface enhances heat transfer efficiency by creating the steam fingers that enlarge the heat transfer area. Moreover, the development of steam fingering at the steam chamber edge can control steam-assisted gravity drainage (SAGD) chamber growth which is directly related to the oil production rate.



Final remarks

- The results show that taking advantage of instability at the chamber edge can enhance thermal efficiency by enlarging the heat transfer interaction area at the chamber edge.
- The instability is more focused at the top of the chamber where the bitumen is above steam.
- On the evolution of thermal fingers, fingers are regularly spaced and interact at the edge of the steam chamber.
- Superfine grid simulation is required to resolve finger evolution.

TECHNOLOGICAL-ECONOMIC-SOCIAL-ENVIRONMENTAL RESERVOIR SIMULATION TOOLKIT: TESERS TOOLKIT

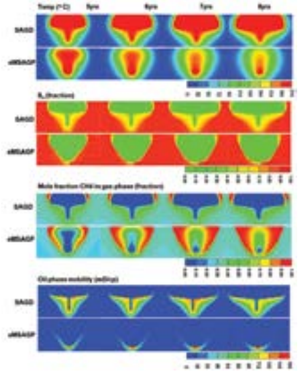
Ian Gates, Getachew Assefa

Background

Development of reservoir recovery processes requires scale-up from lab-scale testing to field scale execution. This is typically done by using reservoir simulation where lab-scale models can be matched to calibrate input parameters (physical properties, multiphase flow, etc.) and then scaled-up to field scale to obtain projections of the technology at field scale. In this subproject, the research team will build lab-scale and ultra-resolved field-scale reservoir simulation models, based on real geological data, to provide field scale performance of new recovery processes. The novelty of the approach will be an integrated modelling environment linking together commercial reservoir simulators as well as optimization tools and multi-scale analysis together with life cycle assessment and impact assessment tools. Within the project, low emission and potentially zero-emission recovery processes for oil sands reservoirs will be researched. These include new well architectures and completion designs, new injection strategies, and steam-additive and solvent-based recovery processes. As new designs emerge, a social life cycle analysis will be conducted to examine the technology from a social and technoeconomic viewpoint.

Research strategy

The research strategy includes the construction of ultra-defined oil sands reservoir models that are realistic with heterogeneity represented at small (tens of centimeters) to large (kilometer) scales. These models will be used with new well architectures, e.g., fishbone wells, and completion designs, e.g., flow control devices, to understand how to lower the steam-to-oil ratio of steam-assisted gravity drainage (SAGD). Solvent and additive co-injection will be examined to determine



methods that will significantly lower the steam-to-oil ratio. Solvent-rich low temperature or cold processes will also be explored for low and near zero emissions recovery process designs.

Desired outcomes

The desired outcomes from this project are a set of new designs that have significantly lower emissions intensity than that of existing steam-based recovery technologies such as SAGD with similar or better economic performance. Social barriers to the use of the new designs will also be examined.

Technological-economic-social-environmental reservoir simulation toolkit: TESERS Toolkit

Technoeconomic analysis of energy systems, value added petrochemical products and climate resiliency of electricity systems

Eranda Bartholameuz
Postdoctoral Fellow

Introduction

Dr. Eranda Bartholameuz, PhD, is working in collaboration with the Canadian Energy Research Institute on analyzing and modelling energy systems. Specific research includes evaluation of the Canadian oil and gas sector regulatory framework, analyzing value-added pathways for petrochemicals, distributed power generation, and climate resiliency of electricity systems.

Results

Eranda developed a new risk analysis strategy for the Canadian oil and gas sector regulatory framework using the capital asset pricing model and modelled the cost of regulatory delays for Canadian oil and gas projects.

In addition, Eranda modelled the energy potential of biomass and municipal solid waste for distributed generation in Canada and modelled a scenario-based analysis for impacts of different value-added petrochemicals on the Canadian industry. Eranda is currently working on recovery pathways for renewable energy sector from COVID-19 impacts and on climate resiliency of electricity systems in Canada.

Final remarks

- Oil and gas sector investment risk is mainly driven by market factors; however, it was also determined that sub-sectors could have different risk levels based on current geopolitical environments.
- Biomass energy technology has potential to be an alternative energy technology for distributed generation. Although general biomass costs seem to be higher, biomass incineration coupled with internal combustion engines proved to be the cheapest technology combination.

Technological-economic-social-environmental reservoir simulation toolkit: TESERS Toolkit

The economic effectiveness of different carbon pricing options to reduce carbon dioxide emissions

A K M Nurul Hossain
Postdoctoral Fellow

Introduction

The accumulation of greenhouse gases (GHGs), and the resulting rise in global temperatures and climate change, are attracting a great deal of attention globally. To limit the adverse impacts, a variety of related efforts to reduce GHGs are available or being developed on the international, national and sub-national levels. Dr. A K M Nurul Hossain, PhD, takes the quantitative approach and analyzes the impact of some major policy initiatives around the globe — the European Union Emissions Trading System (EU ETS), the California (linked with Quebec) Cap-and-Trade System, the British Columbia (B.C.) Carbon Tax System and the Alberta Specified Gas Emitters Regulation (SGER). A K M estimates how these policies affect three major indicators: (1) emissions efficiency, as measured by GDP per unit of CO_2 emissions, (2) economic performance, as measured by real GDP and (3) GHG emissions in those jurisdictions.

Results

A K M takes the difference-in-differences (DiD) approach to analyze the systematic differences between the treatment group (where the policy was implemented) and the control group before and after the implementation of an emission policy. One key advantage of this approach is its ability to identify the treatment effects of a policy from two angles: the cross-sectional difference and the time-series difference. To check the robustness of the analysis, he also conducted a series of placebo tests using fake treatment years.

A K M finds that the EU ETS and the California cap-and-trade have had a robust impact on emissions reduction. In contrast, the B.C. carbon tax and Alberta SGER failed to reduce GHG emissions. Additionally, both EU ETS and California cap-and-trade improved the emissions efficiency while the B.C. carbon tax and Alberta's SGER failed to have any significant impact. Also, only the California cap-and-trade was successful at increasing GDP while reducing emissions. This result confirms the so-called double dividends concept for California cap-and-trade.

Final remarks

- A K M examined whether the carbon management policies in the EU-25, California, Quebec, B.C. and Alberta have been effective in meeting the policy goals.
- The EU ETS and California cap-and-trade contributed substantially to their efforts to decarbonize their economies.
- Both the EU ETS and the California cap-and-trade improved the emissions efficiency while the B.C. carbon tax and Alberta's SGER failed to have any significant impact.
- The B.C. carbon tax had no impact on provincial emissions reduction but had a positive impact on GDP.
- The Alberta SGER failed to reduce GHG emissions.

Technological-economic-social-environmental reservoir simulation toolkit: TESERS Toolkit

Life cycle sustainability assessment of unconventional oil resource development: The case of new versus existing technologies

George Ike
PhD student

Introduction

This project involves using the life cycle sustainability assessment methodology to assess new innovative technologies in the oil sands. George Ike aims to drive sustainability by accounting for environmental, economic and social impacts of the latest low carbon techniques being developed under GRI and comparing the performances with conventional methods. In this project, he intends to find the best way to present the triple bottom line measures in unconventional oil and gas resource development, with emphasis on the social dimension to assess how acceptability and speedy deployment of new methods could be achieved. Specific cases George has started considering are solvent extraction methods and hydrogen production from bitumen.

Results

While the economic benefits derived from the oil sands industry are substantial for Alberta and Canada, the environmental impacts of the industry remain a significant challenge. Several new lower emissions technologies have been developed for oil sands operations. However, historically, the pace of technology implementation has been slow in the industry. George intends to develop a framework to identify and assess various social factors that are working against wider-scale deployment of low carbon technologies in the oil sands. By addressing the social impacts of these technologies, he hopes to underscore the roles of these technologies in the economy of Alberta, thereby enhancing the acceptability and breaking social barriers.

In addition to the social aspects, as part of efforts to decarbonize the oil sands activities, he estimates the carbon footprint of hydrogen production from the oil sands as well as that of solvent extraction methods using life cycle assessment methods. He also examines the utilization pathways for hydrogen coming from Alberta heavy oil.

Final remarks

- Hydrogen production from microwave heating of bitumen provides significant environmental benefits.
- George will develop social and environmental impacts benchmarks to inform regulatory and consumption decisions.
- He hopes to develop criteria for selecting and characterizing new technologies with respect to economic, social and environmental implications.

Technological-economic-social-environmental reservoir simulation toolkit: TESERS Toolkit

Patent analytics for in situ oil sands technology evolution tracking

Aarthi Muthuswamy
Postdoctoral Fellow

Introduction

The objective of the project is to build an intelligent patent analytics toolkit to track the evolution of in situ oil sands technology across various domains and automate the toolkit using keyword search analytics.

Results

Dr. Aarthi Muthuswamy, PhD, developed a steam-assisted gravity drainage (SAGD) specific keyword search engine code and obtained data from 800+ SAGD-related patents from the years 1981-2019. Aarthi tracked key trending technology of solvent and steam injection, as shown in Figure 1. The results show that steam-solvent combinations are one of the consistent technology thrusts arising in the past decade of technology evolution for in situ oil sands recovery process design. Data across 800+ patents was visualized to get a time- and company-wise complete picture. The top ten company contributions were identified based on the trending technology. Aarthi is currently preparing a journal article on patent analytics for SAGD evolution.

Final remarks

- A keyword-based patent search engine was developed to read and analyze patents across in situ oil sands recovery processes, and the engine could be expanded to other applications.
- Steam and solvent injection were the top technology development theme arising from the analytics engine for oil sands recovery processes.
- Information from the patent analytics engine demonstrates that the new technologies are incremental improvements over SAGD.

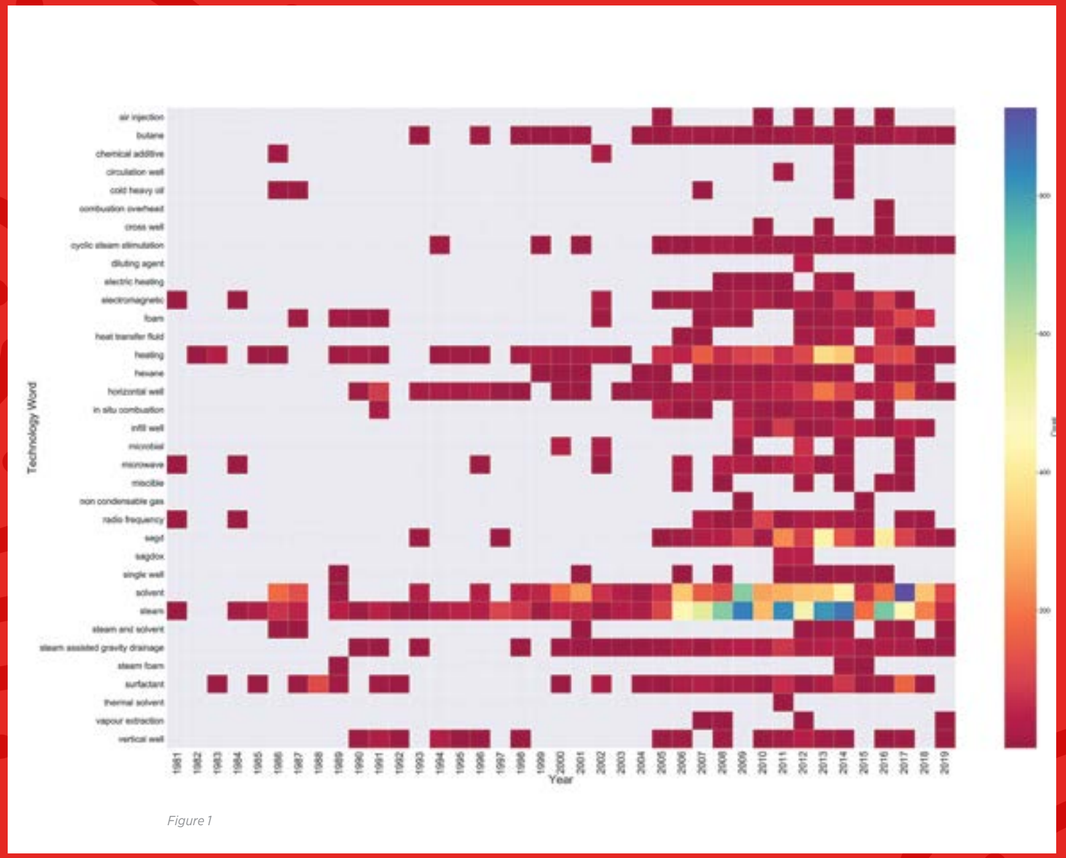


Figure 1

RHEOLOGY IN ENHANCED OIL RECOVERY

Giovanniantonio Natale, Anne Benneker

Background

New technologies to enhance heavy oil recovery are based on injection of gas (e.g., CO_2, CH_4), emulsions, solvents in combination with or instead of water steam. This has shown to reduce emissions and energy consumption related to the oil recovery process. The injection of gas (developing foam in situ) and emulsions are particularly interesting not only from an economic and energetic point of view but also considering the potentialities that these complex systems have on enhancing production and reducing the time lag between injection and production cycles. However, the dynamics of these systems, optimization of their performance and control of their microstructures are still far from achieved.

The rheology of complex fluids, such as emulsions and foams, play a key role in enhanced oil recovery (EOR). Emulsions and foams are non-Newtonian fluids usually showing bulk viscoelastic shear thinning behaviour. Moreover, surface active molecules like low molecular weight fatty acids, naphtenic acids and asphaltenes are usually present within crude oil and affect both the rheological and the physico-chemical behaviour of in situ generated emulsions and foams.

Research strategy

To optimize the EOR techniques, a considerable issue to consider is interfacial rheology. Rheological considerations can be applied at the pore level of porous media. Here, emulsions and foams are supposed to fill the pores by capillary rise dynamics. Although shear-thinning fluids show a faster penetration as compared to Newtonian ones, the picture of capillary penetration of complex fluids is still unclear and more work is needed to elucidate this problem. In the case of emulsion and foams, wetting, and more in general surface chemistry, hydrodynamics and confinement play a major role in establishing both the droplets behaviour and the oil recovery performance.

To analyze this complex system, this project employs a combination of bulk and interfacial rheology, and fluorescent microscopy coupled with a home-made setup to create flat (liquid-gas or liquid-liquid) interfaces for microstructural analysis.

Desired outcomes

This project aims to link interfacial properties of asphaltene stabilized emulsions and foams to bulk rheological properties to explain their pore level properties, to explore the effect of nanoclay particles on the interfacial properties and microstructures of asphaltene molecules at interfaces, and to investigate the effect of additives (nanocrystal cellulose) on the interfacial and bulk properties of asphaltene stabilized emulsions.

Rheology in enhanced oil recovery

Rheology and microstructure of CNC based liquid crystalline phases and the effect of magnetic field

Ashna Rajeev
Postdoctoral Fellow

Introduction

The objectives of this project are the preparation and rheological characterization of the liquid crystalline (LC) droplets of cellulose nanocrystals (CNC) in water in a continuous oil phase. Dr. Ashna Rajeev, PhD, mainly focuses on tuning the LC assembly of CNC nanoparticles in the droplets with changes in the external magnetic field. This finds applications in the stabilization/destabilization of emulsion droplets as well as in the transport and delivery of materials in the core of the droplet. She is also studying LC CNC-polymer composite nanoporous flexible films for the design of smart membranes with tuneable porosity for the selective removal of gas molecules.

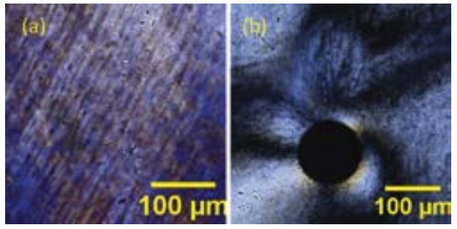


Figure 1

Results

Ashna has started working on the preparation of the liquid crystalline phase by dispersing CNC in water. Her current research focuses on the study of flow properties of the liquid crystalline dispersion of CNC by means of polarization optical microscopy (POM) and rheometer. The preliminary rheological results showed a sol-gel transition as the concentration of CNC increased. She observed that the CNC dispersions form a cholesteric liquid crystalline phase (Figure 1a), at concentrations above seven weight per cent (wt%) with a twisting birefringent pattern around discontinuities (Figure 1b). This is very interesting in terms of the changes in the birefringent pattern under confined conditions such as emulsion droplets. She observed that the CNC films retain the liquid crystalline ordering even after drying. This property can be used in the preparation of flexible polymer films by dispersing CNC particles in a suitable polymer like polyethylene glycol (PEG).

Final remarks

- CNC dispersions form a cholesteric liquid crystalline phase at high concentrations.
- The liquid crystalline ordering in the CNC film, even in the dried film, and in the PEG composite film were the same.
- The rheological studies show a sol-gel transition with an increase in the concentration of CNC.

SOLVENT-ADDITIVE (NANOPARTICLE/EMULSION) DYNAMICS AND INTERACTIONS

Qingye (Gemma) Lu

Background

In both aqueous or non-aqueous heavy oil and bitumen recovery processes, solvent and additives are required to facilitate oil solid separation and to increase the recovery efficiency. For example, in chemical enhanced oil recovery process, surfactant is added to water to increase oil recovery through reducing oil solvent interfacial tension and modulating rock wettability, polymer is added to control the mobility of injected water. Understanding the dynamics and interactions between solvent and additives is critically important.

Desired outcomes

The research will provide better understanding on the dynamics and interactions between these additives with solvent, which will lead to improved and optimized industrial processes encompassing from oil sands extraction to solvent recovery. The research will also lead to the development of additives with higher efficiency, lower cost and better environmental profile. Additionally, the research will train highly qualified personal with critical technical skills.

Research strategy

The research has four main focuses: (1) Understanding the dynamics and interactions between the additives with solvent under various conditions using advanced analytical techniques, herein solvent including aqueous and non-aqueous solvent, additives including any chemicals which are functionally important in heavy oil and bitumen recovery as well as related processes. (2) Producing additives using environmentally friendly starting materials in combination with integrated and efficient processes. (3) Characterizing the physical and chemical properties of these additives. (4) Testing the functions of these additives under industrially relevant conditions.

Solvent-additive (nanoparticle/ emulsion) dynamics and interactions

Microfluidic synthesis of 2D graphene oxide based nano particles and their application in energy and environmental field

Md. Mehadi Hassan
PhD student

Introduction

Md. Mehadi Hassan aims to synthesize a unique physicochemical property containing antibody conjugated two-dimensional graphene oxide (2D-GO) and biopolymer-based nanoparticles via a microfluidic platform. Investigating the efficacy of this microfluidic synthesis route is also the key aspect of this research work. A microfluidic system offers reaction with high-throughput screening, feasible and rapid experiments on small sample scale and provides a lot of information at the microlevel production. The main challenges of this project are to design and fabricate an efficient integrated microfluidic device and to investigate the microstructural aspects of synthesized nanoparticles.

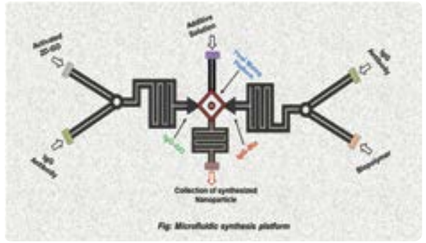


Fig: Microfluidic synthesis platform

Results

The feasibility of peptide bond formation between antibodies (e.g., IgG) on the surface of 2D-GO and three-dimensional (3D) biopolymer sodium alginate will be tested in this research project. Incorporation and optimization of proper additives (e.g., crosslinking reagent: ethylenediamine and poly-ethyleneimine, transition metal salt) into the antibody conjugated 2D-GO and biopolymer would potentially assist to get the expected physicochemical property containing a solidified crosslinked flexible nanocomposite. The expected enhanced mechanical and microstructural properties of fabricated nanoparticles could be explained based on the surface textural analysis, multiple functionality and degree of active pathogen detection sites on the surface of nanoparticles. It is anticipated that contribution of 2D-GO, 3D-biopolymer and suitable additives could enhance the mechanical and sensing performance of nanomaterials. Overall, the outcome and the novelty of this work would be an important steppingstone in the field of microfluidic technique for nanoparticle synthesis.

Final remarks

- Scope of nano to millimetre scales synthesis, cost-effectiveness, rapid and efficient reaction, multistep chemistry, as well as integrated separation steps make microfluidics a powerful platform for synthesizing a wide variety of nanomaterials.
- Antibody conjugated single atom thick 2D-GO and 3D-biopolymer-based nanomaterials would be the better choice for mechanically enhanced nanostructured materials for diverge level of pathogen detection.
- This research output could potentially assist to understand the fundamental aspects and impacts of synthesizing nanomaterials in microfluidic platform.

Solvent-additive (nanoparticle/ emulsion) dynamics and interactions

Development of novel materials and microfluidic techniques for interfacial science analysis

Maryam Razi
Postdoctoral Fellow

Introduction

In this project, Dr. Maryam Razi, PhD, aims to develop novel materials and microscale technologies with the application in the water/wastewater sector. A model 3D-printed modified Scheludko-cell (MSC) has been implemented to monitor the efficiency of adsorption of heavy metal ions in the aqueous environment. The integration of electrochemical sensing with 3D printing technology and microfluidic technology is yet another objective of this project. The proposed technique can be used for ultrasensitive detection of pathogenic bacteria in water/wastewater media. Development of novel materials such as a plant-based de-oiling agent from lignin which is a by-product of the wood industry will also be targeted as part of the project. Most of chemicals formulated to be used as demulsifiers and reverse emulsion breakers (REB) are formulated from toxic phenolic resins with ethylene oxide (EO)/propylene oxide (PO) added in their structures. The aim is to develop novel environmentally-friendly demulsifiers/reverse emulsion breakers and to understand their interfacial behaviour at oil-water interfaces.

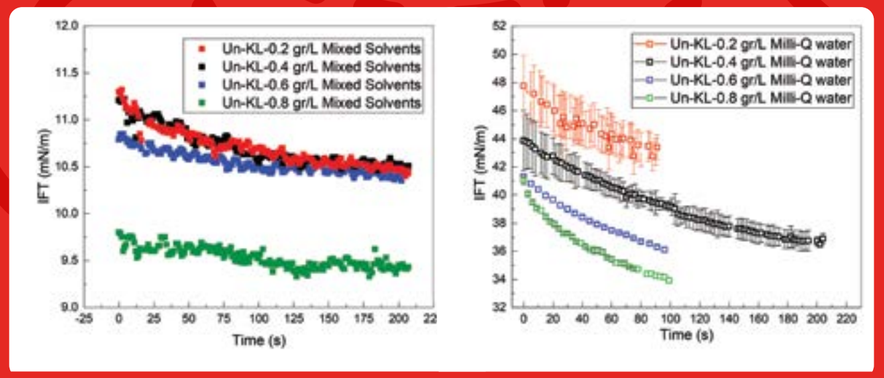
Results

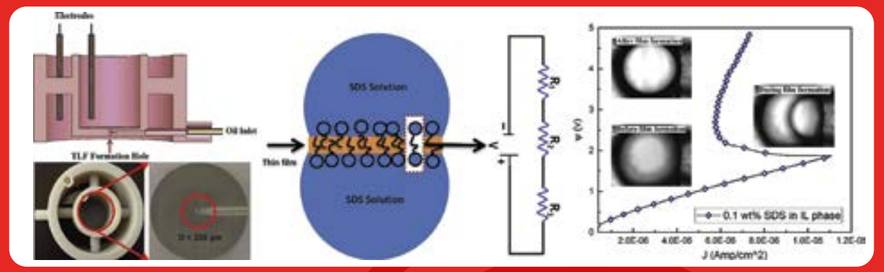
Maryam has worked on the development of 3D-printed microscale technologies for heavy metal ion detection. The systemic study of a thin liquid film (TLF) formed between the aqueous phases has been performed. The conductivity of the formed TLF has been obtained as concentration of heavy metal ion present in aqueous phase.

She has published several articles in international journals outlining some of the obtained results of her work in interfacial science, microfluidic technologies, thin liquid films and adsorption analysis at micro and nanoscales.

Final remarks

- As environmental pollution and its effect on human health is the predominant factor in the development of new generations of tomorrow's technological developments, understanding the underlying mechanisms for environmental pollutions or toxic chemicals and their effects on human health is of vital importance.
- Development of novel materials and microscale/microfluidic technologies made it possible to detect, monitor and treat the impurities in water/wastewater using very low sample volumes and in a fraction of seconds.





Solvent-additive (nanoparticle/ emulsion) dynamics and interactions

Production of synthesis gas via dry reforming of methane: Fundamentals and applications

Rufan Zhou
PhD student

Introduction

The aim of Rufan Zhou's proposed research is the development of an efficient technology to convert CO_2 via dry reforming of methane (DRM) to produce value-added products. There are two main knowledge gaps associated with the DRM process which hinder its industrial application: catalyst deactivation and the high energy requirement for the CO_2 conversion reaction. This proposed research is designed to bridge these gaps by using novel catalysts to mitigate coke formation, followed by high-level heat recovery and plant-wide optimization. This study will allow Canada to meet major milestones required to reduce GHG emissions and transition to a lower carbon economic system.

Results

Rufan's research project is still in the preliminary stage and he has not obtained results yet.

Final remarks

- A novel Ni/CeO_2 catalyst for dry reforming has been successfully synthesized.
- A novel catalyst with good long-term performance with less coke formation is desirable.
- The reason of coke formation will be investigated, and the effectiveness of distinct catalyst fabrication methods will be examined.
- Rufan expects that the novel catalyst obtained from this project will broaden the future application of DRM.

ENZYME ENHANCED OIL RECOVERY

Jinguang Hu, Hector de la Hoz Siegler, Ian Gates

Background

Biodesulfurization (BDS) a process recruiting microorganisms to remove the sulfur content in crude oil. A limited species of microorganism has been identified containing enzymes to oxidize and remove the sulfur from thiophene compound. BDS process removes the sulphur without losing the caloric value of the fuel, and it is conducted at ambient conditions. Therefore, BDS could be taken as a complimentary method, or even could be developed as an eco-friendly and costless alternative to the current industrial desulfurization process in fuel refinery. However, the BDS process has many limitations. Firstly, the expression of the enzymes is supressed by the sulfur compounds. Secondly, the enzyme catalytic BDS is a complex process containing four enzymes and other co-factors. Besides, the final product of BDS shows inhibitory effects to the enzymes involved in the catalysis. The research team is interested in optimizing the BDS catalysis via different approaches, including developing a BDS assay only with purified recombinant enzymes, and building up a hybrid catalytic system by combining the enzymes with catalysts.

Research strategy

To develop a cell-free BDS assay with purified recombinant enzymes, the first step is to collect purified enzymes from bacteria E. coli overexpression system. Currently, all four enzymes that are required for the BDS are cloned into bacteria over-expression vectors. After obtaining purified recombinant enzymes, the enzyme conducted catalysis could be performed in test tubes and the reaction could be monitored by high-performance liquid chromatography (HPLC) as using dibenzothiophene (DBT) as the substrate. With the cell-free enzymatic assay, more work could be focused on improving the BDS efficiency through protein engineering, enzyme immobilization, or via the combination of inorganic catalysts.

Desired outcomes

This research aims to obtain recombinant BDS enzymes from *E. coli* overexpression system, and to develop a cell-free enzymatic desulfurization approach with purified recombinant enzymes. Additionally, it is expected to contribute to the creation of several research papers and patents, and to the collaboration with industrial partners.

Enzyme enhanced oil recovery

Development of a cell-free enzymatic assay in biodesulfurization efficiency evaluation

Jia Li
Postdoctoral Fellow

Introduction

Biodesulfurization (BDS) is discovered in a limited species of microorganisms in which enzymes are recruited to remove the organo-sulphur content from the crude fuel. The BDS process removes the sulphur without losing the caloric value of the fuel, and is conducted at ambient conditions. Thus, BDS could be developed as an eco-friendly and costless alternative to the current industrial desulfurization process in fuel refining. However, the BDS process has many limitations, including the complex catalysis (four enzymes are needed) and the product-inhibitory effects to the catalysis. To optimize the BDS process for its future application in the industry, a cell-free enzymatic assay to measure the BDS efficiency is necessary.

Results

It is necessary to collect pure enzymes in soluble forms to establish a cell-free enzymatic assay. To obtain soluble proteins of good yield, all four enzymes that are required for the BDS are cloned into the bacteria over-expression vector. One of the four enzymes has a good yield of soluble protein. The other three enzymes are aggregated at the current induction condition. The induction conditions, bacteria strains and expressing vector should be reviewed and modified for an optimized result. Other chemicals needed for the BDS, or co-factors, are being procured. Crude oil samples are used to establish the enzymatic assay. With the cell-free enzymatic assay, more work could be focused on improving the BDS efficiency through protein engineering and enzyme immobilization or via the combination of inorganic catalysts.

Final remarks

- All four enzymes that are required for BDS process are induced to be expressed with good yield in bacteria.
- Protein induction conditions and purification methods need to be modified to obtain soluble protein.

CARBON RECYCLING IN OIL SANDS RECOVERY

Md Golam Kibria, Samira Siahrostami, Ian Gates

Background

Oil sands account for 10 per cent of Canada's GHG emissions and about 0.15 per cent of global GHG emissions. In oil sands processes, natural gas is commonly burnt to produce steam for subsequent injection into the wellbore for enhanced recovery. Other energy-intensive processes include steam methane reforming (SMR) for producing the hydrogen needed to upgrade heavy crude oil. All these steps release GHGs into the atmosphere. Therefore, the Oil sands industry is challenged to find ways to reduce CO_2 emissions while enhancing the efficiency of the recovery and upgradation processes. One of the promising pathways to substantially reduce GHG emissions is integration of carbon capture and utilization (CCU) with oil sands processes, e.g., steam assisted gravity drainage (SAGD). Analysis suggests that by 2025 nearly 90 per cent of the GHG emissions can be reduced via SAGD with CCU.

Research strategy

The proposed project aims to develop electrochemical pathways to substantially reduce CO_2 emissions from oil sands processes as informed by techno-economic and life-cycle assessment. Starting from fundamental understanding of the reaction mechanisms, this project aims to develop novel catalyst and electrodes as well as design a high throughput electrocatalytic system to convert CO_2 to methane (CH_4) and organic solvents. The produced CH_4 can offset the required CH_4 for the upstream steam generation and SMR processes. In addition, the proposed project will develop electrochemical production of renewable hydrogen that can replace carbon intensive steam reforming process used in oil sands industry.

Desired outcomes

The core outcome of this project is environmental stewardship, specifically, the decarbonization of the oil sands industry while maximizing the efficiency of recovery and refining processes.

Carbon recycling in oil sands recovery

Electrochemical reduction of CO_2 into valuable chemicals

Muflih Arisa Adnan
PhD student

Introduction

The principal objective of Muflih Arisa Adnan's project is to reduce CO_2 emissions via electrochemical reduction of CO_2 (ERC). The ERC enables conversion of CO_2 into valuable chemicals using electric power. This strategy takes advantage of the availability of renewable electric power in the future. Muflih is designing theoretically efficient transition routes from the conventional system into a fully electrochemical process via ERC. Additionally, he has discovered several potential materials as efficient and robust catalysts for ERC and has studied the reaction mechanism of ERC using different catalysts materials.

Results

Muflih has performed techno-economic analysis of several possible power-to-methanol routes and has established the performance target of CO_2 electrolysis so that the power-to-methanol synthesis route becomes economically and environmentally competitive in the near future. Using thermodynamic analysis, he studied the integration of biomass gasification and electrochemical reduction of CO_2 in order to mitigate the accumulated CO_2 emissions in the atmosphere. He considered the advantage of biomass feed as the natural capture of CO_2 from the air and provided the range of oxygen equivalence ratio in the biomass gasification in order to obtain the optimum performance in terms of CO_2 emission reduction. Moreover, he evaluated the comprehensive economic feasibility of the power-to-methanol route by utilizing electricity from the concentrated solar photovoltaic and CO_2 from a direct air capture plant.

Final remarks

- The current density and energy efficiency (technical factor) and electricity price (external factor) have significant influence on the economic feasibility of power-to-methanol routes.
- The oxygen equivalence ratio in the biomass gasification delivers substantial effect on the CO_2 emission reduction in the integrated biomass gasification and electrochemical reduction of CO_2.
- Capital and operating costs of concentrated solar photovoltaic technology have significant effect on the economic feasibility of the process.
- Muflih's next step is to develop the catalyst for CO_2 electrolysis to increase the CO_2 electrolyzer performance including the current density and selectivity. He will also provide the reaction mechanism of the reaction in the corresponding catalysts.

Carbon recycling in oil sands recovery

Electrocatalytic conversion of carbon dioxide and methane to high-value chemicals

Tareq Al-Attas
PhD student

Introduction

The electrochemical carbon dioxide reduction reaction (CO_2RR) has been regarded as a promising strategy to obtain high-value products and concomitantly offset CO_2 emission. Tareq Al-Attas is working on converting carbon dioxide and methane to high-value chemicals through electrochemical conversion. He is developing new approaches to use organometallic compounds as electrocatalysts bridging heterogeneous and homogeneous catalysis for reducing CO_2.

Results

The economic feasibility of CO_2RR relies on the development of highly selective and efficient catalysts operating at a high current density. Tareq has developed a way of increasing the selectivity towards carbon monoxide production from carbon dioxide through ligand engineering of metal-organic framework catalysts. Two different azolate functional ligands — 1,2,4-Triazole (Calgary Framework-20, CALF-20) and 2-Methylimidazole (zeolitic imidazolate framework-8, ZIF-8) — were investigated for CO_2RR. Experimental findings show that CALF-20 is reporting the highest faradaic efficiency of Zn-based MOFs for CO production.

Final remarks

- Tareq concluded that ligand engineering in Zn-based metal-organic frameworks would develop highly selective and efficient catalytic materials to catalyze the electrochemical reduction of CO_2 to CO.
- Experimental results, aligned with ab initio calculations, show that CALF-20 is a more favourable catalyst for CO_2RR than ZIF-8.

Carbon recycling in oil sands recovery

Investigation of the catalytic mechanism of amorphous ruthenium oxide for the electrochemical reduction of CO_2

Santiago Jimenez Villegas
MSc student

Introduction

The CO_2 reduction reaction (CO_2RR) holds great promise as an alternative, carbon-neutral, method for the production of fuels. In this project, Santiago Jimenez Villegas works on investigating electrocatalysts for the conversion of CO_2 into useful materials (e.g., methanol). These catalysts are composed of amorphous metal oxides — a class of materials that have been reported to be highly active and product-selective in the CO_2RR. The project combines both experimental and computational analyses that will not only identify superior catalysts but also elucidate reaction mechanisms at play, ultimately leading to more rational catalyst design principles.

Results

Santiago has synthesized amorphous ruthenium oxide (RuOx) thin films via photochemical metal-organic deposition (PMOD) and near infrared driven decomposition (NIRDD) methods. Early characterization indicates the films are X-ray diffraction (XRD) amorphous. X-rays produced by synchrotron radiation at the Canadian Light Source (CLS) was also used to characterize the RuOx films. The data is currently in the processing stages. Designs and fabrication of an H-cell are being finalized in order to test the catalytic activity of the RuOx films.

Additionally, Santiago has modelled amorphous RuOx by ab initio molecular dynamics (MD), as implemented in Vienna ab initio Simulation Package (VASP). Density functional theory (DFT) calculations are carried out on the amorphous RuOx model to explore surface reactions and possible pathways that lead to the formation of different products during the CO_2RR. Preliminary calculations show a favoured CO_2 to methanol reaction on RuOx.

Final remarks

- Product formation and efficiency of the RuOx catalyst will be monitored once fabrication of the H-cell is complete.
- The processed data acquired at the CLS will provide valuable insights into both oxidation states and local structure of the RuOx catalyst. These results will then be used to more accurately model the amorphous films.
- Promising results obtained from early DFT results indicate a favoured conversion of CO_2 to methanol.
- Connecting the results from both experimental and computational studies will allow the research team to gain a deeper understanding into the reaction mechanisms involved in amorphous metal oxides for CO_2RR. The deliverable is more rationally designed catalysts in the future.

Carbon recycling in oil sands recovery

Catalyst design by computational chemistry

Mohammadreza Karamad
Postdoctoral Fellow

Introduction

This project aims to develop new catalysts for a wide range of renewable energy-related technologies using atomic-scale approaches. Examples include electrochemical reduction of CO_2 to valuable chemicals, electrochemical reduction of nitrates to ammonia, the oxygen evolution reaction, and the oxygen reduction reaction. Dr. Mohammadreza Karamad, PhD, uses theoretical tools, in particular density functional theory (DFT), to reveal trends in electrocatalytic activity and selectivity of different electrochemical reactions. Moreover, Mohammadreza is using data-driven methods, such as machine learning, to accelerate new material discovery.

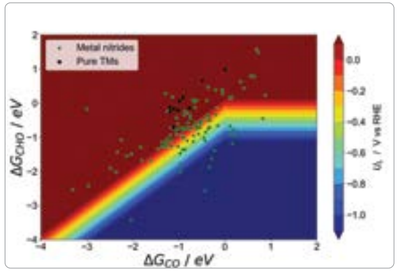


Figure 1

Results

A high-throughput DFT screening study on heteroatom-doped transition metal nitrides for designing efficient electrocatalysts for the electrochemical reduction of CO has been conducted. In this project, different important criteria for designing promising catalysts for the electrochemical reduction of CO such as high activity, high selectivity towards desired products and high stability at the electrochemical conditions have been investigated. The results revealed that metal nitrides and heteroatom-doped metal nitrides as potential electrocatalysts for CO reduction reaction as depicted in Figure 1.

In another project, a novel method for encoding materials information in conjunction with a unique machine learning architecture called the Orbital Graph Convolutional Neural Network (OGCNN) has been developed to enable high-accuracy predictions of material properties. Using the OGCNN, significant prediction accuracy has been achieved over previously developed material representation and machine learning methods. Figure 2 shows the comparison between the prediction accuracy for the formation of an alloy dataset using different methods.

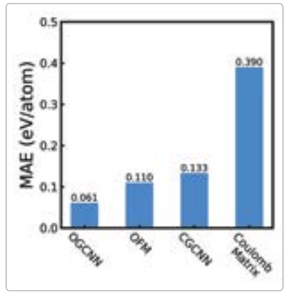


Figure 2

Final remarks

- Metal nitrides are a promising class of materials for CO electrochemical reactions by exhibiting desired activity, selectivity and stability.
- In developing proper descriptors for material representations for data-driven material discovery, inclusion of features that consider the interactions between the constituent elements of materials plays a key role.

Carbon recycling in oil sands recovery

Ligand engineering in ZN–based metal–organic frameworks for electrochemical reduction of CO_2 to CO

Xue Yong
Postdoctoral Fellow

Introduction

The electrochemical CO_2 reduction reaction (CORR) represents a promising way of converting atmospheric CO_2 to useful chemicals. However, CO_2 is extremely stable and inert. It requires large thermodynamics and kinetic energy barrier to reduce CO_2 while competing with hydrogen evolution reaction in aqueous electrolytes. Therefore, highly efficient and selective electrocatalysts are crucial in this endeavour. Zeolitic imidazolate frameworks (ZIF), which are constructed by self-assembly of metal ions and imidazole (2-Methylimidazole) ligands, having versatile structural topologies, have exhibited promising activity in CO_2RR electrocatalysis. Dr. Xue Yong, PhD, aims to improve the CO_2RR electrocatalyst ability and to understand the mechanics of ZIF structure by ligand engineering.

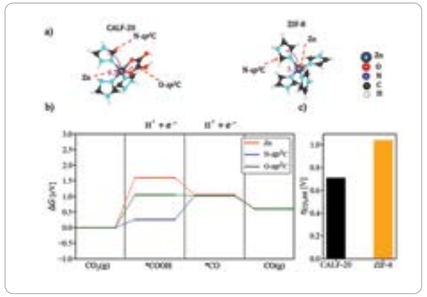


Figure 1

Results

ZIF structure with two different ligands — 1,2,4-triazole (CALF-20) and imidazole (ZIF-8) — have been investigated, depicted in Figure 1a. Zn(II) in CALF-20 lose 1.27 electrons to bidentate oxalate ligand while Zn(II) in ZIF-8, lose less electrons (1.17 electrons) to imidazolates. Therefore, introducing the CO_2 in ligand promotes stronger charge transfer. Analysis of the free energy diagram, shown in Figure 1b, indicates that formation of *COOH intermediate is the potential determining step. For both metal-organic frameworks (MOFs), the adsorption free energy of *COOH over the Zn(II) centres coordinated with the organic ligand in the frameworks is highly endergonic due to fully occupied three-dimensional orbitals in zinc. Formation of *COOH sp_2 C over the bidentate oxalate ligand in the CALF-20 is thermodynamically less favourable than that over the triazolate sp2 C. Thus, the azolate sp_2 C atoms are the most active catalytic site. The calculated free energy of *COOH is 1.109 electron volt and 0.261 electron volt for ZIF-8 and CALF-20, respectively.

Final remarks

- DFT results suggest engineering ligands through introduction of the C_2O_2 bridge promotes stronger charge transfer and formation of stronger zinc-nickel iconic bonds and nickel-carbon bonds in CALF-20.
- Xue found that formation of *COOH intermediate is the potential determining step for the CO_2RR to CO for both MOFs.
- CALF-20 is more active than ZIF-8 as a CO_2RR electrocatalyst. The significantly less *COOH adsorption free energy in CALF-20 can be attributed to more charge transfer in the sp_2 carbon atoms in its triazole, induced by the bidentate oxalate ligand, which facilitates formation of *COOH.

LIFE CYCLE ASSESSMENT AND MULTI-OBJECTIVE OPTIMIZATION OF OIL SANDS OPERATIONS

This project is conducted by the University of Calgary Technology Assessment and Coordination Team (TACT)

Joule Bergerson, Parissa Mirjafari, Getachew Assefa, Ian Gates

Background

Life cycle assessment and mathematical modelling and optimization tools are employed to identify the most desirable technology path from extraction of bitumen to producing refinery products in terms of minimum cost and minimum greenhouse gas emissions (GHG).

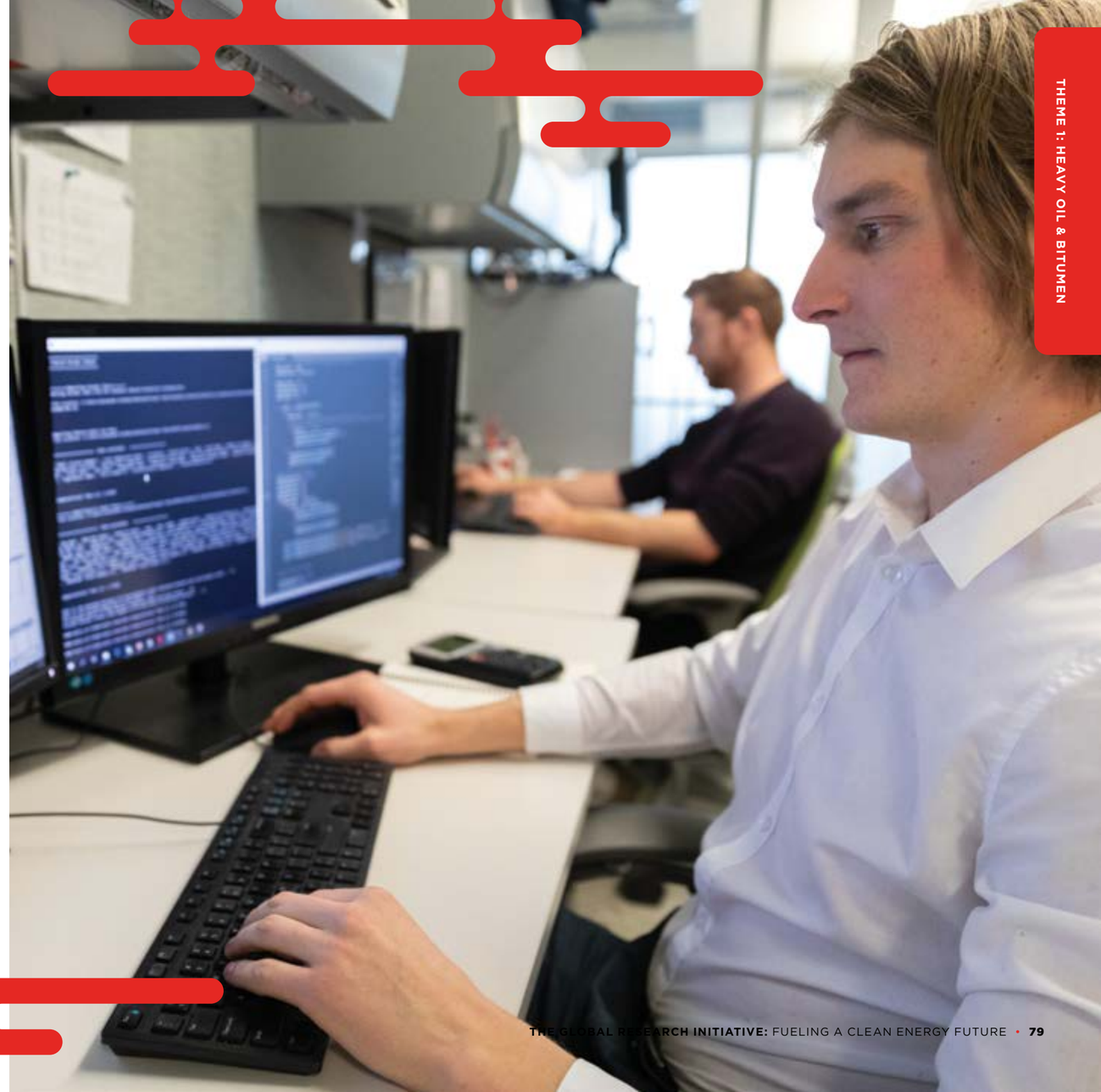
Research strategy

In this project, technology options in oil sand activities including the technologies used for extraction, dilution, upgrading, partial upgrading and refining are investigated. Sensitivity analysis will be conducted to determine the technological and economic conditions under which the emerging technologies (e.g., new partial upgrading technologies) will become viable options for the oil sands industry.

Desired outcomes

This analysis will inform oil sands operators about the technology alternatives that can potentially increase the competitiveness of oil sands products to crude oil markets by reducing the supply chain cost and life cycle emissions of oil sands operations. In addition, results of this analysis can help oil sands producers pursue innovative technology ideas in the oil sands industry and understand the long-term effects associated with the use of existing and emerging oil sands technologies. This analysis will inform investment decision making in the oil sands industry by providing insights about technology pathways in the oil sands operations.

The mathematical model developed here combines life cycle and optimization techniques to create a tool that can evaluate the competitiveness of emerging oil sands technologies (when required data is available for the emerging technology) with respect to economic and environmental criteria. Results of this analysis will provide insights for decision makers in the oil sands industry about emerging technologies. These technologies are in early stage process development and are facing uncertainty due to the lack of performance and cost data comparisons in academic and industrial publications with existing technology pathways.



Life cycle assessment and multi-objective optimization of oil sands operations

Evaluating oil sands technologies using life cycle assessment and mathematical optimization

Zainab Dadashi
PhD student

Introduction

In this project, technology options in oil sands activities including the technologies used for extraction, upgrading, partial upgrading and refining are investigated using life cycle assessment and optimization tools. Oil sands production pathways with minimum GHG emissions and maximum profit through the entire supply chain are identified and the sets of conditions that make each technology a competitive option are determined. Sensitivity analysis is conducted to determine the technological and economic conditions under which the emerging technologies (e.g., new partial upgrading technologies) will become viable options for the oil sands industry.

Results

There is a large overlap between the ranges of profit and well-to-wheel (WTW) GHG emissions generated by different oil sands production pathways when variability and uncertainty of input parameters are considered. Therefore, the choice of the most profitable or the least GHG-intensive oil sands production pathway significantly depends on how the inputs variability and uncertainty are characterized. The results show that solvent assisted extraction technologies can improve the economic and environmental performance of oil sands production under a wide range of input assumptions. Another emerging technology, partial upgrading, is shown to be more competitive than traditional upgrading technology in terms of total cost and total GHG emissions under certain combinations of technological and economic conditions.

Final remarks

- A techno-economic framework that evaluates existing and emerging oil sands production pathways is required to inform oil sands operators about the technology alternatives that can potentially increase the competitiveness of oil sands products to crude oil markets by reducing the supply chain cost and life cycle GHG emissions of oil sands operations.
- Identifying and quantifying the trade-offs between the economic objective function that considers the total cost of delivering oil sands products to market (e.g., gasoline and diesel) and the environmental objective function that considers the impacts associated with delivering these products using different technology pathways when additional industry constraints are added to the analysis helps inform investment decisions in oil sands operations.

Life cycle assessment and multi-objective optimization of oil sands operations

Life cycle triple bottom line sustainability performance space: The case of unconventional oil and gas resources

Marwa Hannouf
Postdoctoral Fellow

Introduction

The successful implementation of technologies depends not only on technical and environmental aspects but also on social and economic factors. The purpose of this research is to use the life cycle sustainability assessment method to create a triple-bottom-line space, shown in Figure 1, of unsustainability conditions, defining the thresholds for technologies to meet on the three dimensions of sustainability. Using this space, Dr. Marwa Hannouf, PhD, is going to assess the performance of technologies under development in Theme 1 and work on improving their performance so they can all fit in the sustainability space, be socially desirable, have the lowest impact environmentally and be economically cost-effective.

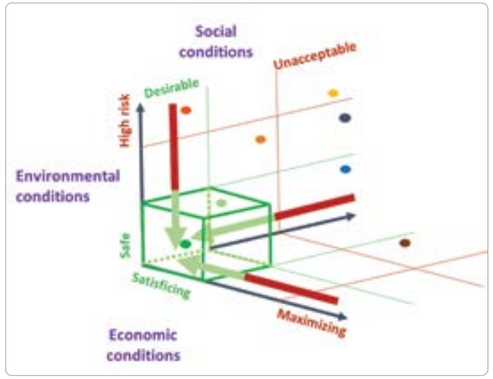


Figure 1

Results

Marwa developed an approach using social-life cycle assessment to identify social areas that need to be legislated by policy makers in Canada, in Alberta and in the oil and gas sector to enforce adequate social conditions for successful implementation of oil and gas technologies in Alberta. In addition, Marwa has conducted a workshop for technology developers in Theme 1 to brainstorm potential social aspects associated with the technologies under development. She believes this workshop was a major step to familiarize the research group with this new topic. On the other hand, Marwa found that current incremental improvements in SAGD operations in Alberta are not enough to achieve reductions in GHG emissions. She identified environmental, economic, and social factors affecting cleaner technology adoption in the industry. She proposed policy-insights to accelerate deployment of cleaner-extraction technologies in oil sands developments and thus, achieve a sustainable energy industry. She published some of these results in articles in peer-reviewed journals and presented at international conferences.

Final remarks

- Marwa has concluded that cleaner technology adoption is highly impacted by social barriers. Her next step is the ongoing development of a method to quantify social aspects in general and in connection to technologies.
- She has found that a reconsideration of oil sands — policy, technology development and social impacts — from a sustainability point of view is required for a sustainable energy industry.
- Marwa has concluded that a triple bottom line perspective is needed for improving the performance of technologies and thus, accelerating their adoption. The next step is to identify thresholds for technologies to meet on the three dimensions of sustainability.

THEME 2: TIGHT OIL & GAS

Research on tight oil and gas resources (Theme 2) has built upon well-established industry partnerships to address two grand challenges: imaging and controlling hydraulic fracturing and enabling small-footprint recovery from low-permeability reservoirs. Integrated solutions are focused on a set of big questions: Can we mitigate and manage risks of induced earthquakes? Can we improve hydrocarbon recovery efficiency while reducing resource utilization and sequestering greenhouse gases (GHGs)? How can we assess and reduce environmental impacts?

The induced seismicity team has accelerated commercialization of risk-based software focused on characterizing critical fractures and developing a validated predictive framework calibrated using data analytics. The fracture-surveillance team has deployed the first-ever field prototype for a multicomponent distributed acoustic sensing system and has delivered an industry short course on machine learning in geophysics. Enhanced-recovery research teams have advanced the understanding of adaptive asynchronous CO_2 huff and puff processes and developed novel optimization strategies for water alternating gas (WAG) processes. Research teams investigating environmental impacts have collaborated in an injection experiment to quantify the fate of methane in groundwater, developed recommendations for groundwater monitoring, conducted life cycle assessments for tight oil and gas development and developed a highly competitive scalable mobile methane sensing system for emissions detection, quantification and reduction.

Prof. David Eaton is the lead of this theme, and Lydia DiCaprio is the Research Associate. Other University of Calgary faculty members involved in the projects under Theme 2 are Profs. Joule Bergerson, Steven Bryant, Shengnan (Nancy) Chen, Zhangxing (John) Chen, Christopher Clarkson, Ke Du, Ian Gates, Hersh Gilbert, Chris Hugenholtz, Kristopher Innanen, Apostolos Kantzas, Donald Lawton, Steve Liang, Brij Maini, Bernhard Mayer, Sudarshan (Raj) Mehta, Tatyana Plaksina, Per K. Pedersen, Jeffrey Priest, Alejandro (Alex) Ramirez-Serrano, Cathryn Ryan, Roman Shor, Rick Tofani, Daniel Trad, Milana Trifkovic, Benjamin Tutolo, Kristen van de Biezenbos and Jennifer Winter.

CAN WE MITIGATE AND MANAGE RISKS OF INDUCED SEISMICITY?

Research Team 1: **David Eaton**, Hersh Gilbert, Per Pedersen, Mirko van der Baan (UofA), Japan Trivedi (UofA), Ryan Schultz (AER)

Research Team 2: **David Eaton**, Shengnan (Nancy) Chen, Jeffrey Priest, Mirko van der Baan (UofA), Japan Trivedi (UofA), Shawn Maxwell (Industry), Pat McLellan (Industry)

Background

Induced seismicity from hydraulic fracturing has galvanized public attention. It is estimated that regionally detectable earthquakes are triggered for only 0.3 per cent of hydraulic fracturing operations. Induced earthquakes occur on pre-existing faults that are critically stressed. However, case studies indicate that faults most readily identified and mapped using classical approaches are typically not activated by hydraulic fracturing. Instead, problematic faults are typically cryptic.

Research strategy

To address the issue, a two-part approach is being undertaken. Firstly, novel procedures for identification and mapping of critically stressed faults in areas of unconventional hydrocarbon development are being investigated. One approach to this problem uses disparate types of evidence including microseismic data, frac hits and outcrop analogues, with the goal of predicting how hydraulic fractures connect to faults and the probability of slip on a pre-identified fault. Another approach uses local structural attributes from 3D seismic data to identify the distribution of faults, from which a 3D geomechanical model is built. Secondly, a novel computational tool is being developed to simulate induced seismicity at spatial scales of millimetres to 10s of kilometres and at timescales of seconds to months. This computational toolbox will aid in producing quantitative mitigation and response plans by combining reservoir-simulation methods with advanced geomechanical and seismological computational tools. The hydraulic fracturing process is simulated based on a geomechanical model. In addition, fluid flow in the hydraulic fractures is coupled with the geomechanical model to determine the activation mechanism of the identified faults.

Desired outcomes

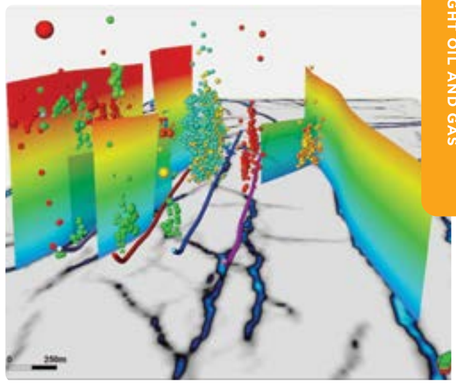
An anticipated outcome of identification and mapping of critically stressed faults is more reliable pre-treatment risk assessment, which will have direct economic impact for industry operations. Additionally, the development of a computational tool will enable creation of a science-informed decision workflow for management of induced seismicity. The activation mechanism of the identified faults will be recognized, which can help regulate the stimulation job size of the hydraulic fracturing operation, such as the injection volumes of fracturing fluid and the injection pressure.

Can we mitigate and manage risks of induced seismicity?

Gang Hui
PhD student

Introduction

A thorough literature review of the hydraulic fracturing-induced seismicity has been conducted. Gang Hui's research concentrates on a case study in Western Canada to investigate the relationship between hydraulic fractures and induced seismicity. He is working on an integrated approach that combines geology, geomechanics and hydrodynamics to quantify the fault activation due to hydraulic fracturing. He is also investigating the mitigation strategy of reducing seismic hazards in Western Canada.



Results

A case study was used to demonstrate the applicability of the integrated method. Four north-south-oriented faults were interpreted and the half-length of hydraulic fractures was calculated. The calculated results of the flow-geomechanics model were in good agreement with the actual induced seismicity spatially and temporally. Three types of triggering mechanisms were determined to account for hydraulic fracturing-induced seismicity, including hydraulic fractures propagation, the hydrology connection between hydraulic fractures and a fault, and connections of hydraulic fractures with the natural fractures around the fault. The injection rate could be decreased to mitigate risks of future seismic events.

Gang has published one article in the *Journal of Petroleum Science and Engineering* and two conference papers in American Rock Mechanics Association (ARMA) and Society of Petroleum Engineers (SPE) meetings, respectively.

Final remarks

- The coupled flow-geomechanics approach was proposed to characterize the activation of faults.
- Three types of triggering mechanisms were determined to account for hydraulic fracturing-induced seismicity.
- The injection rate of fracturing fluid could be decreased to mitigate the risks of aftershocks.

Can we mitigate and manage risks of induced seismicity?

The stochastic characterization and modelling of discrete fracture networks for induced seismicity assessment

Scott McKean
PhD student

Introduction

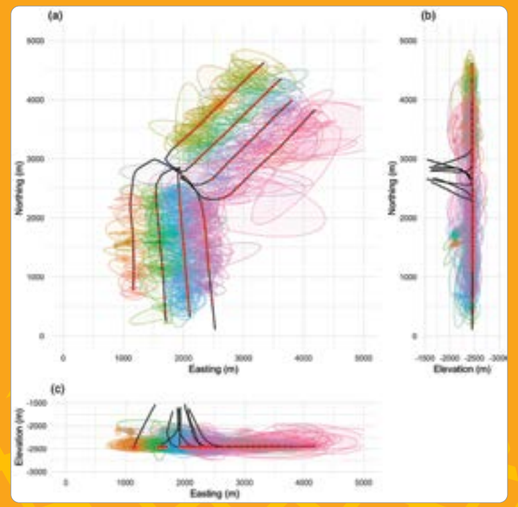
Scott McKean is applying unsupervised machine learning and image processing techniques to characterize small- and large-scale fracture networks using outcrop surveys and microseismic data. A geostasitical assessment of regional rock properties was also conducted to quantify necessary geomechanical parameters for estimating the response of the subsurface to hydraulic fracturing. This data is integrated stochastically to produce a robust discrete fracture network model for the assessment of induced seismicity potential.

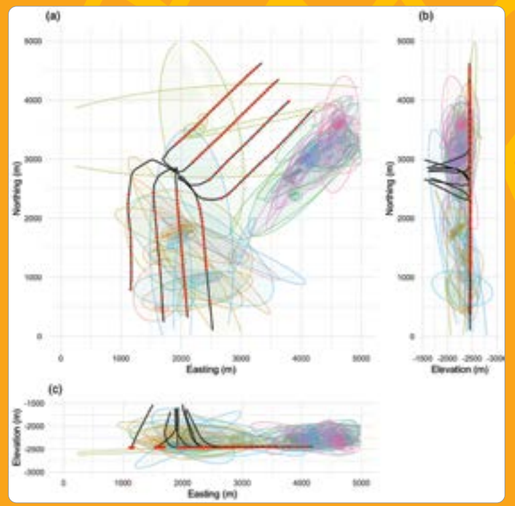
Results

Scott developed an unsupervised learning algorithm that couples the physics of hydraulic fracturing with Gaussian mixture models to identify meso-scale fracture networks within a microseismic point cloud. An outcrop study was conducted on an outcrop equivalent of the Duvernay Formation — an induced seismicity prone reservoir in Central Alberta. This outcrop study included detailed photogrammetry and characterization of geomechanical behaviour and mechanical heterogeneity. These geomechanical properties were combined with public data to create a geostatistical model of rock properties across a large portion of the formation. Image segmentation techniques were used to extract heterogeneity and discrete fracture network characteristics from the photogrammetric surveys of both the Duvernay Formation and its underlying strata, which is suspected to be a major contributor to the induced seismicity risk. The classification algorithm is now being applied to several other microseismic datasets and being integrated into a holistic discrete fracture network model.

Final remarks

- The efficacy of hybrid physical-statistical models for microseismic assessment has been demonstrated.
- Scott has conducted a unique survey and testing of a Duvernay equivalent outcrop in order to quantify discrete fracture networks and geomechanical properties.
- Machine learning and image segmentation techniques have been applied to extract difficult-to-obtain information from disparate data sources.
- Scott is integrating the above information into a holistic understanding of discrete fracture networks in the Duvernay Formation.





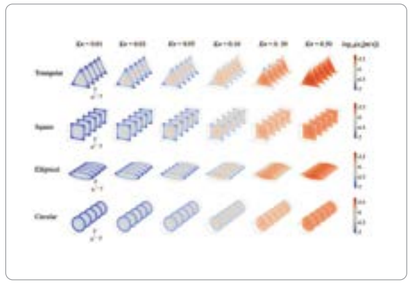
Can we mitigate and manage risks of induced seismicity?

Characterizing the shale rock properties through analytical and experimental methods

Yu Pang
Postdoctoral Fellow

Introduction

Various unified gas flow (UGF) and apparent permeability models have been proposed to characterize the complex gas transport mechanisms in shale formations. Such models, however, are typically expressed as combinations of multiple gas flow mechanisms so that they cannot predict the gas velocity profile. In this project, Dr. Yu Pang, PhD, developed a novel approach to predict the gas velocity profile in the entire Knudsen number (Kn) regime for circular and noncircular (i.e., square, triangular and elliptical) nanochannels and investigate the effects of cross-sectional geometry on gas transport in nanoporous shale.



Results

Yu found that the cross-sectional geometry has a significant influence on the mass flow rate and velocity profile in nanochannels. The predicted mass flow rates for the nanochannels with identical hydraulic diameter decrease with the cross-sectional geometry in the sequence of ellipse, equilateral triangle, square, circle. However, the ranking of velocity profiles for such nanochannels, which is governed by the cross-sectional geometry (aspect ratio), also varies with Knudsen number.

Final remarks

- Yu has developed a novel approach that is able to predict the gas velocity profile for the synergetic gas transport (i.e., advection, gas slippage, bulk diffusion and Knudsen diffusion) in nanochannels with different cross-sectional geometries. This approach provides insights into the characterization of gas transport behaviours in nanoporous shale.

Can we mitigate and manage risks of induced seismicity?

Understanding and mitigating induced seismicity risk in the Kiskatinaw area, B.C.

Rebecca Salvage
Postdoctoral Fellow

Introduction

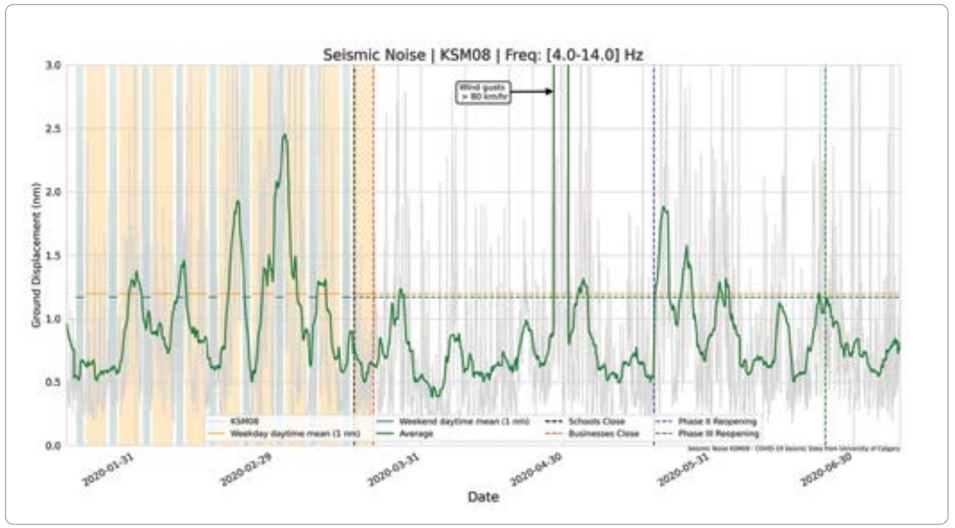
In January 2020, a new dense array of 15 seismometers was installed in the Kiskatinaw area, B.C., to closely monitor hydraulic fracturing activities in near real-time. With such a dense array of sensors, research in this area is better able to characterize fault dynamics and evolution in relation to ongoing unconventional resource development in the area. This is done through better constraints on earthquake locations, magnitudes and seismic source characteristics. With unprecedented seismic quiescence due to COVID-19 as resource development halted, Dr. Rebecca Salvage, PhD, has been able to better understand the background seismic noise, dynamic triggering of events from teleseismic events, and draw conclusions on latent/natural seismicity occurring as a result of increased stresses due to ongoing resource development.

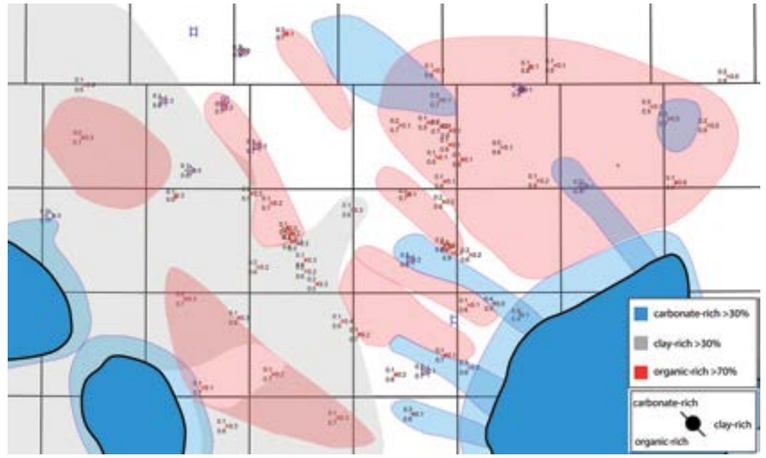
Results

Near real-time detection of seismicity in the Kiskatinaw area has allowed Rebecca to closely monitor when and where hydraulic fracturing operations are occurring. High-precision location analysis suggests seismicity forms distinct linear patterns in relation to these operations; Rebecca is further investigating the occurrence of latent seismicity in these situations that may occur within highly stressed formations at depth following the withdrawal of fluids. Rebecca is also in the process of using locations, magnitudes and other source characteristics to try to distinguish between the different types of operations ongoing in the Kiskatinaw. Furthermore, Rebecca has been able to detail changes in seismic noise in relation to human activity during the COVID-19 pandemic. A significant drop in noise when the government lockdown was implemented can be observed, as well as several large jumps in the noise level, in particular relating to when the government began reopening businesses.

Final remarks

- High precision locations, magnitudes and source characteristics have allowed Rebecca to closely monitor unconventional reservoir development in the Kiskatinaw area, B.C.
- Rebecca is working closely with the regulator to try to determine distinguishing characteristics for seismicity from different types of operations in the area.
- Unprecedented seismic quiescence due to COVID-19 has allowed Rebecca to determine the background noise in the Kiskatinaw area and determine changes in the noise levels related to pandemic activity (e.g., lockdown measures and reopening of businesses).


Seismic Noise | KSM08 | Freq: [4.0-14.0] Hz
Wind gusts > 80 km/hr
Ground Displacement (nm)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
KSM08
Weekday daytime mean (1 nm)
Weekend daytime mean (1 nm)
Average
Schools Close
Businesses Close
Phase II Reopening
Phase III Reopening
2020-01-31
2020-02-29
2020-03-31
2020-04-30
2020-05-31
2020-06-30
Date


carbonate-rich >30%
clay-rich >30%
organic-rich >70%
carbonate-rich
clay-rich
organic-rich

Can we mitigate and manage risks of induced seismicity?

Geological influence over geomechanical characteristics of the Duvernay Formation in the Kaybob area, AB, Canada: Implications for field development and induced seismicity mitigation

Marco Venieri
PhD student

Introduction

Marco Venieri's goal is to understand the correlation between geological and geomechanical characteristics of the Duvernay shale at the core, wireline log and three-dimensional (3D) seismic scale. The aim of his project is to gain knowledge about which factors exert the most influence on the geomechanical behaviour of shales undergoing hydraulic fracturing treatment. This has applications for unconventional reservoir field development as well as induced seismicity mitigation.

Results

Using core-focused studies as a starting point, Marco has developed an innovative workflow capable of correlating rock characteristics and their geomechanical properties at the wireline log scale. This relaxes the requirement to rely solely on cores for the geological and geomechanical characterization of unconventional shale plays. Additionally, Marco was able to extend this relationship between geology and geomechanics to 3D seismic. This has been extensively discussed in three separate papers and 15 conference presentations over the last three years. This workflow has been practically applied to corroborate an induced seismicity dataset published as a paper in *Science Advances* of which Marco is co-author (Eyre et al., 2019). In this research, estimation of mineralogy and geomechanics from wireline logs provided a geological framework to the estimated hypocenter location, happening right at an important mineralogical — and thus mechanical — subsurface boundary.

Additionally, Marco is focusing on the quantification of geological and geomechanical heterogeneity in organic-rich shales at the centimetre-scale to address the issue of upscaling operations when integrating core data with bigger scale datasets such as wireline logs and 3D seismic. He is currently building variograms to preserve important geological and geomechanical boundaries during the upscaling operation and evaluating their impact on reservoir simulation.

Final remarks

- Geological and geomechanical properties of organic-rich mudstones can be successfully tied at the core, wireline logs and 3D seismic scale being aware of the differences and assumptions behind each methodology.
- Estimation of mineralogical and geomechanical properties of unconventional shales from wireline logs can successfully be integrated with core data in areas with poor core control for more detailed reservoir characterization.
- Depending on mineralogy, fabric and diagenetic characteristics, shales can reach an extremely high degree of geological and geomechanical heterogeneity at the centimetre-scale. Preserving geomechanical boundaries when upscaling the data is crucial to generate a scientifically correct 3D reservoir model.

GREEN HYDRAULIC FRACTURING FLUIDS

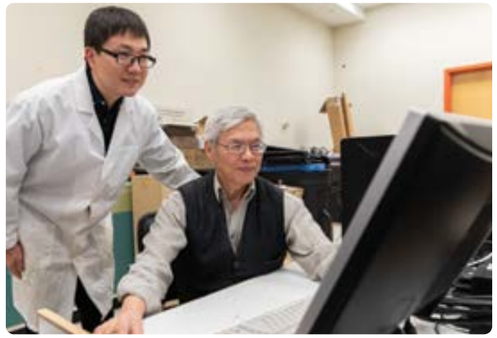
Shengnan (Nancy) Chen, Tatyana Plaksina, Brij Maini, Jeffrey Priest, Joule Bergerson, Sudarshan (Raj) Mehta, Zhangxing (John) Chen, Per Pedersen

Background

Hydrocarbon liquid-rich shale (LRS) reservoirs are currently the hottest targets for unconventional reservoir development in North America. The most common means of exploitation is primary recovery through horizontal wells which are completed in multiple stages along the well with massive (usually water-based) hydraulic fracture stimulation treatments (multi-fractured horizontal wells or MFHWs). Continuing at increased scale will place additional stress on resource utilization and an increase in unforeseen/unintended environmental incidences, such as hydraulic fracturing-induced seismicity. MFHWs completed in unconventional resources may also provide a solution to mitigate greenhouse gas (GHG) emissions. Recently operators have piloted the use of MFHWs as both fluid (water and gas) injection and production wells in an effort to improve oil recovery in LRS reservoirs. Hypothetically GHG injection (e.g., CO_2) through MFHWs may be used to not only increase oil recovery, but sequester GHGs. However, CO_2 storage and transport mechanisms in LRS are poorly understood, as are the hydrocarbon recovery mechanisms.

Research strategy

In this project, several avenues have been adopted to address the grey areas which includes the development of improved fracture surveillance and designing "green" hydraulic fracturing fluids. Additionally, evaluation and manipulation of the fundamental controls on hydrocarbon fluid recovery and GHG storage using GHGs as the injected fluid are being considered. Moreover, schemes to co-optimize CO_2/lean gas enhanced oil recovery (EOR) and sequestration are being explored.



Desired outcomes

Combinations of methodologies for seismic acquisition will be validated in laboratory studies and in field scale trials. Other related projects will be generating methodologies for pre-processing data and for producing properly parameterized full-waveform inversion (FWI) algorithms; here, field and lab validation and prototyping will be focused on.

Green hydraulic fracturing fluids

Zheng Li
PhD student

Introduction

The project intends to understand hydraulic fracturing and validate fracturing models by using laboratory-scale experiments to physically simulate the hydraulic fracturing process as it occurs in the field. This involves understanding the fracturing mechanics and calculations and performing finite element analysis of multi-stages hydraulic fracturing in Abaqus.

Results

The main outcomes from the research so far have been: (1) successfully visualizing the fracture growth in formations; (2) radial fracture modelling and matching; and (3) natural fracture activation and relevant stress field calculation using finite element method (FEM) software.

Final remarks

- The experimental results show that hydraulic fracturing tends to grow perpendicular to the minimum principal stress direction. In relatively close stress fields, a branched fracture will generate, especially in the near wellbore zone.
- Stress field analysis in FEM proved that the hydraulic-induced fractures will change stress fields nearby and make them extremely complex. Therefore, in multi-stage fracturing or repeated fracturing processes, choosing an appropriate space between each fracturing stage is quite important.

IMPROVED RESERVOIR CHARACTERIZATION BY ADVANCED SEISMIC PROCESSING

Kristopher Innanen, Daniel Trad, Don Lawton

Background

Currently, there is limited ability to create well-resolved subsurface models of distributions of fractures, fluids, viscosities, etc., in unconventional reservoirs, though in principle the seismic data used to monitor these reservoirs contains this information and possibly more. An important and yet incompletely answered scientific and engineering question concerns whether and how this information can be unambiguously extracted from the complex seismic waveform information. Theoretical frameworks exist, in the form of full-waveform inversion (FWI), but data preparation, acquisition, preprocessing and parameterization, all aspects of FWI which must be selected a priori, are difficult to optimize.

Research strategy

This research will provide technology for tracing frac fluid distribution in the subsurface/improved hydraulic fracture design and monitoring. By partnering with industrial collaborators, well characterized but challenging datasets will be used as the backdrop for developing practical workflows and methodologies of multicomponent elastic full-waveform inversion.

Desired outcomes

The workflow and parameterization conclusions, a systematic survey of FWI results, a range of industrial datasets and datasets acquired for purpose by the research group will be the key outcomes of this project. Combinations of acquisition parameters, waveform inversion parameterization, data preprocessing (“waveform consistent”) will be of practical industrial and basic scientific value.

Improved reservoir characterization by advanced seismic processing

Ali Fathalian
Postdoctoral Fellow

Introduction

Dr. Ali Fathalian, PhD, aims to develop a derivation of a system of equations to show velocity and attenuation of acoustic waves in a medium with transverse isotropy (TI). This project is concerned with seismic modelling in viscoacoustic tilted transverse isotropic (TTI) media. This type of rheology has received far less attention than acoustic TTI media. Acoustic anisotropic modelling has been the most widely used constitutive law in seismic exploration. Ali finds the analysis of viscoacoustic TTI media relevant by deriving the equations for a general viscoacoustic TTI medium with anisotropy in velocity and attenuation.

Results

He introduced the theory and derives a system of equations for seismic modelling in attenuating TTI media. In Figure 1, he shows numerical examples to demonstrate the validity of the method and the conditions for guaranteeing the stability of the computations for a discretization with the finite-difference method. The examples displayed an excellent agreement between this approach and an alternative implementation for modelling seismic waves in TTI media with attenuation. Figure 2 shows that the proposed approach is stable in media with a strong contrast in the physical properties and cases with varying degrees of complexity. A modelling example with realistic geologic complexity showing the usefulness of this approach for applications in seismic modelling, imaging and inversion was also developed.

Final remarks

- A new approach for modelling waves in viscoacoustic TTI media is derived by eliminating the shear components of the constitutive law and introducing anelasticity with the standard linear solid (SLS) model.
- There is a very good agreement between this approach and an alternative implementation for modelling seismic waves in viscoacoustic media with anisotropy.
- The proposed approach is stable in media with a strong contrast in the physical properties and models with varying degrees of complexity.
- The proposed approach is useful for seismic modelling, imaging and inversion.

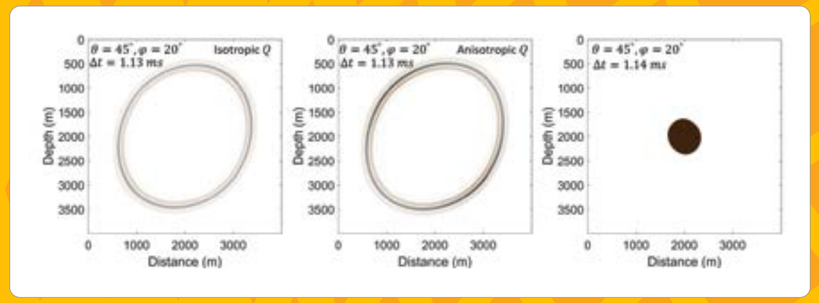


Figure 1

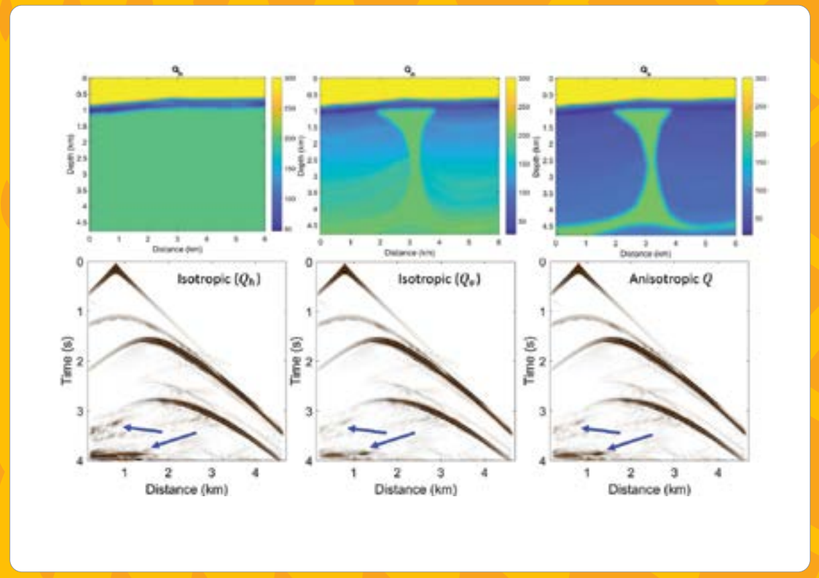


Figure 2

Improved reservoir characterization by advanced seismic processing

Ali Fathalian
Postdoctoral Fellow

Introduction

The key step for seismic structural interpretation and reservoir characterization is delineating faults from seismic images. Dr. Ali Fathalian, PhD, studies fault detection as a binary image segmentation problem. He performed an efficient image-to-image fault segmentation using a convolutional neural network (CNN). The Australian field data indicate that the neural network can predict faults from seismic images much more accurately and efficiently than conventional methods.

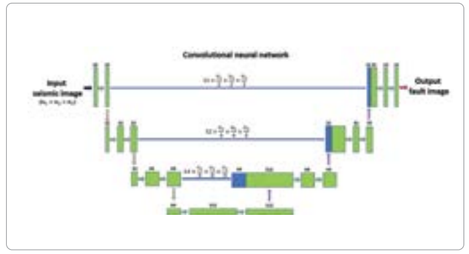


Figure 1

Results

Ali has discussed a convolutional neural network to detect faults from seismic images by considering fault detection as a binary segmentation problem. The network creates seismic images and the corresponding binary fault labeling images are sufficient to train a good fault segmentation network. After training, the network can learn to calculate the main features that are important for fault detection. The convolutional neural network is simplified by reducing the number of convolutional layers. This simplification significantly saves graphics processing unit (GPU) memory and computational time. Figure 1 shows the simplified convolutional neural network for three-dimensional (3D) fault detection. The results show that the trained neural network can predict faults from seismic images accurately and efficiently.

Final remarks

- After training, the neural network automatically learns to calculate the main features that are important for fault detection.
- The neural network can accurately detect faults from three-dimensional (3D) field seismic volumes.
- The neural network saves GPU memory and computational time for training and prediction.

Sustainable hydrocarbon recovery from low permeability reservoirs

Machine learning applied to geophysical data

Marcelo Guarido de Andrade
Postdoctoral Fellow

Introduction

Dr. Marcelo Guarido de Andrade, PhD, aims to develop new machine learning applications to apply to structural geology on seismic sessions, such as faults and fractions. Different deep learning algorithms (CNN, U-net, ResNet, etc.) are used to identify geophysical/geological features in a migrated seismic session to help interpreters to come to conclusions faster.

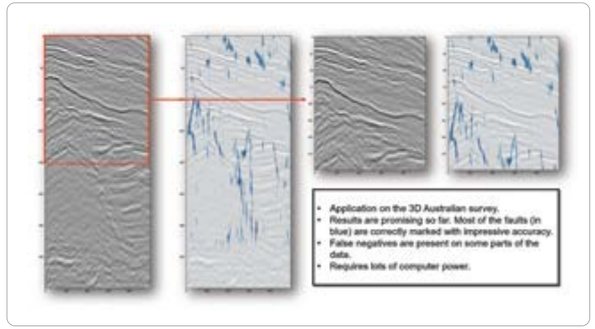


Figure 1

Results

Marcelo is collaborating with Professor Daniel Trad and Postdoctoral Fellow Ali Fathalian to develop a fault detection tool with three-dimensional (3D) approximations. They are applying a U-net deep learning model. This model was trained on synthetic seismic data, and the predictions are done on a 3D offshore seismic survey from Australia (Poseidon 3D Seismic). Figure 1 shows the first promising results, but it requires heavy computer power.

Final remarks

- First results are promising, with a lot of possible areas for improvement, such as deep learning model selection, to feature engineering of the seismic session prior to modelling.
- A two-dimensional (2D) approximation is also under development. It requires less computer power, opening for the possibility to use more complex deep learning algorithms to obtain more consistent results.

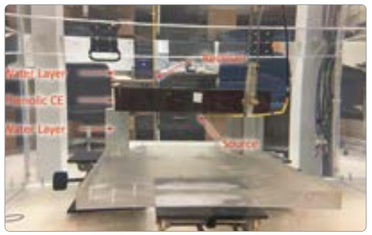
Improved reservoir characterization by advanced seismic processing

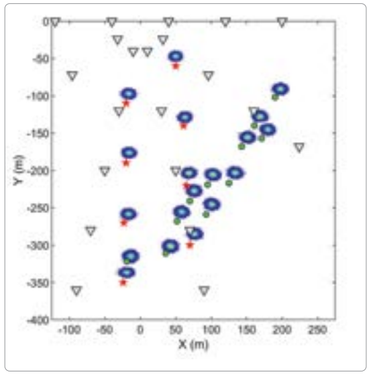
Bayesian inversion for anisotropic parameters and microseismic event locations

Hongliang Zhang
Postdoctoral Fellow

Introduction

Dr. Hongliang Zhang, PhD, focuses on locating microseismic events in anisotropic media, such as reservoirs with a set of vertical aligned fractures in a finely horizontally layered background. He developed a Bayesian algorithm to simultaneously estimate microseismic event locations and anisotropic parameters. In contrast to deterministic inversion algorithms, his approach can provide nonlinear uncertainty quantification by approximating the posterior probability density with an ensemble of model-parameter sets. Hongliang also works with other research staff to validate his algorithms on physical modelling data acquired at the University of Calgary.





Results

Hongliang has implemented the simultaneous Bayesian inversion for horizontal transverse isotropic (HTI) and orthorhombic (ORT) media. The procedure employs Bayesian inference via Markov-chain Monte Carlo sampling with parallel tempering and diminishing adaptation to ensure efficient sampling. His approach was tested with physical modelling data, in which an analog anisotropic layer was built by using canvas phenolic resin (CE) material and a star-like surface array. Results show that, with known origin times, posteriors of all model parameters exhibit Gaussian-like distributions without secondary modes. Whereas, for the case with unknown origin times, posteriors of origin times, event depths and anisotropic parameters exhibit multi-modal features. Numerical simulations indicate that these features could be eliminated by using a large aperture array or including an extra downhole array. The comparison between results using HTI and ORT models implies that the ignorance of vertical transverse isotropy (VTI) caused by horizontal layering in a fractured reservoir may lead to systematic event-location errors.

Final remarks

- The inversion rigorously quantifies parameter uncertainties by treating locations of perforation shots and microseismic events, effective anisotropic parameters and the noise standard deviation as unknown.
- The ORT model is more suitable than HTI to characterize the fractured reservoirs.
- A large aperture of the star-like array and the inclusion of an extra downhole array can both help resolve for stable inversion results.

HOW TO ACCURATELY ASSESS AND SUBSEQUENTLY REDUCE ENVIRONMENTAL IMPACTS OF DEVELOPMENT OF LOW PERMEABILITY HYDROCARBON RESOURCES?

Research Team 1: **Cathryn Ryan**, Chris Hugenholtz, Alejandro (Alex) Ramirez-Serrano
Research Team 2: **Bernhard Mayer**, Cathryn Ryan
Research Team 3: **Bernhard Mayer**, Roger Beckie (UBC), Aaron Cahill (UBC)
Research Team 4: **Joule Bergerson**

Background

The recent expansion of the oil and gas industry into unconventional hydrocarbon reservoirs in North America has generated public concern regarding the potential contamination of groundwater, soils and the atmosphere. One of the primary questions is to what extent, if any, does hydraulic fracturing result in contamination of shallow freshwater and drinking water supplies due to fugitive gas migration or due to flowback fluids containing saline formation waters and chemicals used during hydraulic fracturing? Another key knowledge gap is the extent of greenhouse gas (GHG) emissions, especially methane, into the atmosphere associated with the production of shale gas from unconventional hydrocarbon reservoirs.

Research strategy

In this research, the team attempts to determine the rates and sources of fugitive methane released via surface casing vent flows (SCVF), gas migration (GM) outside of energy wells and more diffusive fugitive gas leakage via measurements and data compilations. Moreover, the team is developing monitoring approaches to assess the potential impacts of fugitive gases and saline waters with chemicals used in hydraulic fracturing on shallow groundwater. The research team also investigates the fate of fugitive gases such as methane and ethane once they enter the shallow groundwater zone. The obtained knowledge will be used to identify the most effective approaches to minimize environmental impacts.

Desired outcomes

As an outcome of this research the rates of fugitive gas emissions will be better quantified and researchers will attempt to identify the locations of highest greenhouse gas emissions. Approaches to reliably assess environmental impacts on shallow water resources will be developed and applied to better quantify the extent of potential environmental impacts. In addition, the attenuation capacity for fugitive methane in aquifers will be determined and quantified. Effective approaches will be developed to minimize environmental impacts by identifying the areas where highest impact can be achieved. This will lead to marketable monitoring technologies and products.

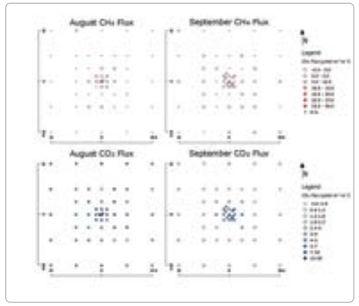
How to accurately assess and subsequently reduce environmental impacts of development of low permeability hydrocarbon resources?

Field investigation of gas migration around a leaky petroleum well

Neil Fleming
MSc student

Introduction

Under the supervision of Dr. Cathryn Ryan, Neil Fleming's research will better the understanding of subsurface behaviour and total emissions of natural gas from a leaking energy well. His project involves a field-based study of the current methods used by the industry for the detection of leaking wells and the monitoring of the spatial and temporal variability of the gas. The outcome of this research will be aimed towards improving scientific and industry-related well testing.



Results

Results from an intensive CO_2 and CH_4 efflux study indicate that migrating gases were concentrated along the well casing, with strong spatial variability around the wellhead. Effluxes varied between greater than 100 micromole photons per square meter per second (µmol photons/m^2 /s) of CH_4 to non-detectable amounts within meters from the wellhead. Temporal evolution of effluxes indicate that migrating gases are controlled by environmental factors such as air pressure and temperature. Short-term variability is also explained by evolution of the migrating gases. Detectable concentrations of methane around the well varied by more than one order of magnitude over the two-week monitoring period, however, the highest measurements always remained consistently above background values. Soil gas compositional and isotopic measurements indicate that a small portion of the methane is being oxidized.

Final remarks

- Flux rates of migrating gases are temporally variable (at several time scales) with apparent environmental controls by wind speed, temperature and barometric pressure.
- This variability will affect both gas movement detection strategies and studies of longer-term variability.
- Gas movement behaviour and efflux rates are different close to versus further from the preferential flow path.
- Most of the gas efflux occurs along a preferential flow pathway.
- CH_4 is being oxidized to CO_2, leading to isotopic shifts and diagnostic gas compositions.
- Total site emissions are estimated to be 0.4 cubic metres CH_4 per day, less than the emissions generated by one cow.

How to accurately assess and subsequently reduce environmental impacts of development of low permeability hydrocarbon resources?

Can we assess impacts on potable waters (groundwater and surface waters) from fugitive gases, saline waters and chemicals used in hydraulic fracturing?

Tiago Morais
PhD student

Introduction

Tiago Morais aims to contribute to the understanding of the fate of fugitive gases in the saturated and unsaturated zones around leaky oil and gas wells, the key processes and mechanisms that govern its transport and attenuation in both dissolved and free phases, and the hydro-biogeochemical implications of fugitive methane invasion into the shallow groundwater zone.

He also aims to improve the understanding of the constraints and opportunities for continuous monitoring of both dissolved and free phase gas in shallow groundwater through near-surface measurements taken from groundwater monitoring wells.

Results

Based on the results from preliminary fieldwork campaigns performed around a leaky well that has been leaking natural gas for more than a decade, Tiago has observed the occurrence of elevated methane concentrations in the shallow groundwater zone around the well, and significant temporal variability in fugitive gas emissions. Future work will involve long-term monitoring of field parameters, water geochemistry and free and dissolved gases at multiple depths in the shallow groundwater zone. It is expected that the results from this long-term monitoring will provide a more comprehensive characterization of the fate of fugitive gases around the leaky oil and gas wells.

Tiago has also found that continuous field parameters can potentially be used as a tool to estimate free phase gas fluxes and identify multiphase flow regimes in groundwater wells. He believes that the development of continuous monitoring tools to accurately detect and monitor the occurrence of free phase gas in the shallow groundwater zone is particularly important in fugitive gas migration studies.

Final remarks

- Gas migration events are heavily concentrated around the oil and gas leaky well and seem to be very episodic.
- The leakage depth and the anisotropy of the geologic medium appear to play a critical role in transporting methane in the shallow groundwater zone.
- There are significant spatial variations in gas concentrations, both laterally and with depth in both saturated (shallow groundwater) and unsaturated zones.
- Long-term monitoring is essential to evaluate the mechanisms that control the transport of dissolved and free phase gas methane and to assess the hydro-biogeochemical implications of fugitive methane invasion into the shallow groundwater zone.

How to accurately assess and subsequently reduce environmental impacts of development of low permeability hydrocarbon resources?

Artificial intelligence for leakage prediction from hydrocarbon wells

Mehdi Rezvandehy
Postdoctoral Fellow

Introduction

The main goal Dr. Mehdi Rezvandehy, PhD, has for his research is to test whether it is possible to predict serious fluid leakages (methane, carbon dioxide, etc.) from hydrocarbon wells without extensive field measurement campaigns. Imperfectly sealed wells accessing hydrocarbon reserves may lead to contamination of groundwater, and soils, and a rise in greenhouse gas emissions. Serious leakages should be detected and fixed to prevent environmental pollution. The challenge is that extensive field tests are costly and time consuming. Therefore, the objective of this research is to train various machine learning and deep learning algorithms for predicting leakage probability for untested wells. The training data is field tests for some energy wells in Alberta operated by Alberta Energy Regulator, shown in Figure 1. Each well has 25 physical properties including age, depth, production/injection history, deviation, etc.

Results

Mehdi first developed a novel technique for imputation of missing well properties such as depth, age, production, deviation and casing size. Uncertainties in missing well property values are quantified and correlations between these properties are reproduced after imputation. He applied a wide range of algorithms. The models were trained and evaluated using existing field test data. The trained models are tested for a never-before-seen dataset, shown in Figure 2. The most reliable model was achieved by aggregating four promising algorithms that resulted in the implementation of a stronger learner: it has sensitivity and accuracy of 73 per cent and eight per cent, respectively (predictor 13).

Figure 3 shows an example of the predicted probability for serious gas leakage associated with 200 random wells in Alberta that have no test data. Verification of the predictions by subsequent field campaigns would be desirable. This work is in process of publication.

Final remarks

- The methodology Mehdi developed can be applied for any producing field to detect the wells with the highest likelihood of fluid leakage without field tests.
- He concluded that the four most-contributing factors for leakage are age, production duration, geological formation and abandonment date.
- Predicting the probability of serious leakage is significantly helpful for cost-effective field test and leads to environmental advantages by prioritizing amendment of the leakiest wells.

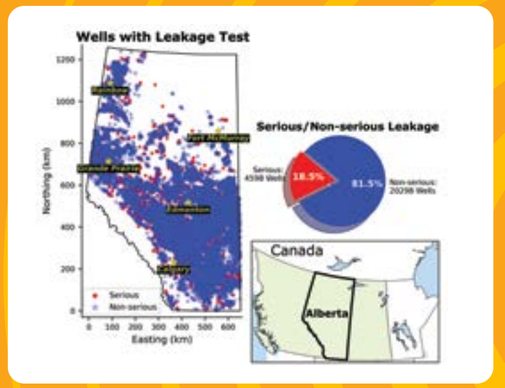


Figure 1

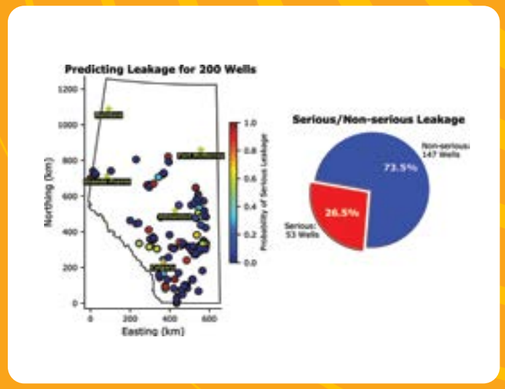


Figure 2

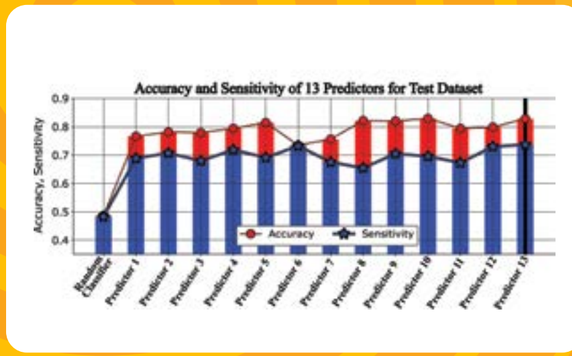


Figure 3

How to accurately assess and subsequently reduce environmental impacts of development of low permeability hydrocarbon resources?

Autonomous sniffer drone

Marshall Staples
PhD student

Introduction

Governments around the world have undertaken initiatives to reduce methane emissions to combat climate change. In the oil and gas industry, fugitive methane emissions are unplanned methane emissions. In order to find methane emissions, Marshall Staples is working on developing an autonomous sniffer drone to localize the source of detected emissions and quantify the leak size. The drone system will be able to solve this problem at scale by surveying multiple facilities in a single flight.

Results

The drone system is autonomous and will generate a flight path that it will follow to ensure that all facilities are searched as quickly as possible while adaptively changing its flight path based on changing wind and environmental conditions. The sniffer drone may also be used by operators of oil and gas facilities to quickly scan and determine which facilities are emitting. This will enable operators to remain compliant with methane emission regulations. The sniffer drone can also be used to check whether oil and gas facilities are compliant with methane emission regulations. The drone system enables a regulator to check multiple facilities with a single flight and quantify the emissions of each facility.

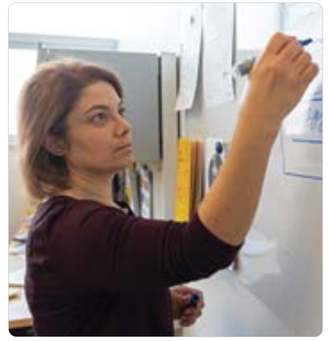
Final remarks

- Fugitive emissions exist and need to be addressed to combat climate change.
- The sniffer drone system can be used to identify and localize fugitive methane emissions.
- The system can be used by the operators of oil and gas facilities as well as regulators.

How to accurately assess and subsequently reduce environmental impacts of development of low permeability hydrocarbon resources?

What are the most effective approaches to minimize environmental impacts? Economics of tight oil and gas production in Western Canada

Julia Yuan
MSc student



Introduction

Julia Yuan's project investigates the costs of tight oil and gas production in Western Canada with the purpose of understanding the economic impacts of this resource in comparison to other Canadian and global energy resources. Western Canadian emissions estimates are used in combination with this research to understand the trade-offs between economics and emissions reductions when recommending effective carbon reduction opportunities. By identifying the drivers of costs and emissions for each tight oil and gas field, unique cost saving strategies can be implemented for fields with high expenditures while prioritizing low emissions. Additionally, the research will assess the cost and environmental benefits of new technologies that are currently employed or potentially applied to tight oil and gas operations.

Results

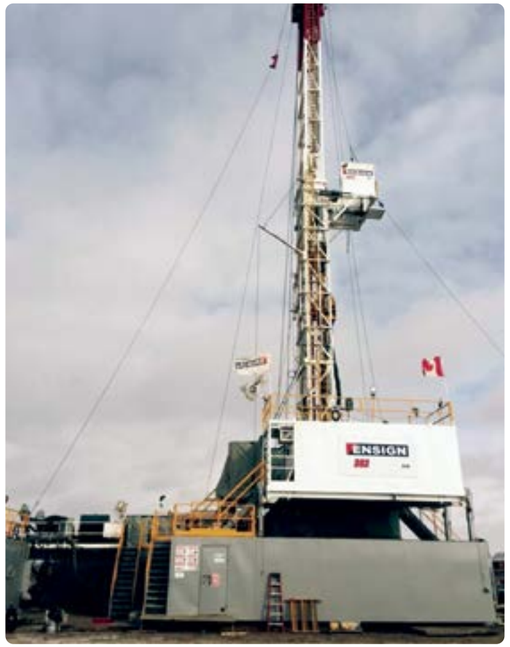
Preliminary results from this research show variations in costs between the Bakken, Cardium, Viking, Lower Shaunavon, Dunvegan and Montney plays. The difference in capital expenditure is influenced by, but not limited to, depth of formation, length of horizontal drilling, number of stages, amount and type of proppant, and amount and type of fracking fluid. Regarding operating expenses, the drivers include, but are not limited to, produced fluid separation and water handling and disposal.

Final remarks

- From the preliminary results, it is evident there are differences between and within each tight oil and gas field.
- Julia will research the relationship between costs and the driving factors for both capital and operating expenditures.
- Julia will also use the relationships identified for each factor to develop a model that determines the well-specific and field-specific costs. Using emissions data for each well and field, the cost and environmental benefits of current operating practices and potential future strategies can be assessed.

METHANE EMISSIONS MONITORING

Chris Hugenholtz, Steve Liang, Ke Du, Encana PTAC, CMCRI CaMI



Background

This project will focus on the research and development required to commercialize a scalable vehicle-based system for measuring methane emissions from upstream oil and gas facilities. Two modes of deployment are achieved with the same hardware: (1) On-pad measurements to locate emitting equipment and guide immediate close-range inspection to identify leaking components, and (2) off-pad measurements to quantify facility-level emissions and flag high emitting facilities for follow-up inspection.

Research strategy

The research strategy consists in the development and testing of software and algorithms, IoT-enabled hardware and in the creation of a cloud-based dashboard for translating raw measurements into actional information leading to emissions reduction.

Desired outcomes

This project already achieved a first live demonstration in December 2019, but a second demonstration is planned for December 2020. Additionally, a performance demonstration in a pilot program is anticipated. The project will include software licensing and the creation of a Startup company.

Methane emissions monitoring

Towards smart methane emissions sensing: deployment optimization of sensor equipped vehicles (SEVs)

Mozhou Gao
PhD student

Introduction

Mozhou Gao aims to advance the operational performance of sensor equipped vehicles (SEVs) by developing optimization strategies. His goal is to incorporate statistical and geospatial techniques to evaluate deployment opportunities and challenges for downwind plume detection and quantification, improve the characterization of methane plumes emitted from oil and gas facilities with measurements from SEVs and explore strategies to enable cost-effective SEV deployment. These research goals will be developed as distinct projects.

Results

Mozhou is focusing on his first project. He has developed a geospatial tool called the Downwind Plume Road Intersection Estimator (DPRIE) to evaluate the suitability of SEVs in different areas of the world. This tool will be used to estimate the suitability of downwind measurement methods based on historical weather data and guide the operation of SEVs based on weather forecast data. Historical weather data will be derived from ERA-Interim reanalysis. Operational forecast data will be derived from the High Resolution Deterministic Prediction System (HRDPS). The PoMELO System will be used to support the operational evaluation and testing by collecting field data.

Current results show that the OTM 33A, the emissions detection, localization and quantification method of SEVs developed by United States Environmental Protection Agency, is not suitable for public road emission quantification in Alberta. Figure 1 shows that the forecast analysis results indicate DPRIE can be used to predict the location of plume crosses for SEVs.

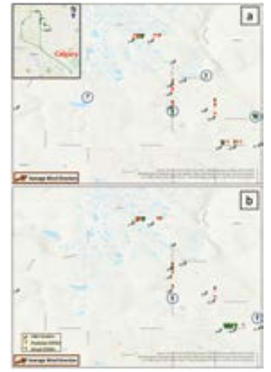


Figure 1

Final remarks

- Mozhou concluded that quantifying emissions from public roads by using OTM 33A is not suitable in Alberta.
- He also found that the spatial requirements of OTM 33A (e.g., the vehicle has to be 20 to 200 metres downwind of the source) are outdated since many vehicles can detect the plume beyond 200 metres, which may be due to the development of sensing technology.
- He also found DPRIE can be used as an operational optimization tool to guide the deployment of SEVs.

METHANE EMISSIONS POLICY AND REGULATION IN CANADA: ASSESSING OPTIONS AND EFFECTIVENESS

Jennifer Winter, Kristen van de Biezenbos, Chris Hugenholtz

Background

Methane emissions are a regulatory challenge for the oil and gas sector and a growing liability for investment in oil & gas. The biggest producers in the world are responding by incorporating methane reduction into business plans and metrics.

The federal government and western provinces have new regulatory schemes aimed at limiting methane emissions from the oil and gas sector and encouraging innovation, but a preliminary review indicates that they are inconsistent and lack harmonization. While there is a growing body of literature on new technologies for methane mitigation, there is very little work on the policy implications of methane regulations, or the efficacy and efficiency of proposed policy actions. This gap serves as the motivation for this project.

Research strategy

Team members will engage industry and regulatory partners throughout the project. These partners will advise and provide feedback on policy and regulatory components of the project. Relationships with these partners are already established through past research and working groups. Connections with industry reps through Petroleum Technology Alliance Canada (PTAC) and Canadian Association of Petroleum Producers (CAPP) will also be leveraged. PTAC leads a number of major methane initiatives on behalf of its industry members and will serve as a node to connect the research project with industry reps engaged in regulatory, policy and economics aspects of methane mitigation.

Desired outcomes

The proposed research agenda has five specific objectives. First, to gain a better understanding of the current set of policies and regulations around methane emissions across Canada. Second, to evaluate the efficiency and efficacy of oil and gas sector methane regulation from a predominantly theoretical standpoint. Third, to evaluate the costs and benefits of different policy actions and regulatory requirements. Fourth, to link policy development and academic policy work to scientific knowledge. Fifth, to mobilize this knowledge and develop a knowledge base for policymakers to use in developing further policy actions.

A minimum of five academic publications are anticipated, conjoint with policy papers as a knowledge mobilization and translation vehicle. This research project will train six highly qualified personnel.

Methane emissions policy and regulation in Canada: Assessing options and effectiveness

Alejandra Garcia
Research Assistant

Introduction

Alejandra Garcia and her research team's goals are to collect methane regulations across select provinces within Canada and to compare them to identify their approaches and their efficacy in the reduction of methane emissions from the oil and gas industry. They also intend to analyze whether equivalency agreements between provincial and federal governments are justified. Moreover, they want to identify which regulatory design is best to facilitate the reduction of methane emissions.

Results

Alejandra has found that the province of British Columbia (B.C.) was granted federal equivalency because it exceeded the emissions reductions target set by the federal government on the province and because B.C. established a right to require investigations of alleged offences in its legislation. Additionally, she has noticed that regulatory design varies across provinces and compared to the federal government. While the federal government and Saskatchewan's regulations seem to be results based, the regulations employed by B.C. seem to be more prescriptive. Finally, she has looked into different types of regulatory design and their benefits and pitfalls to later compare these to the regulatory design behind the methane regulations employed within Canada.

Final remarks

- There is no consensus within legal academia as to which regulatory design or theory is best, and whether the best available technology standard is the most effective in reaching greenhouse gas reductions outcomes. Her next step is to narrow down the more effective regulatory designs.
- B.C. regulations seem to be more general than those enacted by the federal government, yet, according to Environment and Climate Change Canada, B.C. will exceed the federal government's emission outcomes.
- Saskatchewan's regulations rely on the industry's ability to innovate and meet the methane reduction standards.

Methane emissions policy and regulation in Canada: Assessing options and effectiveness

Victoria Goodday
Research Associate

Introduction

This project aims to provide an independent academic assessment of the efficacy and efficiency of different policies, regulations and technologies for managing methane emissions. The objective is to inform policies to meet Canada's emissions reduction goals and simultaneously enable responsible resource development. Victoria Goodday is working with Research Associate Dr. Sarah Dobson to identify the sources of anthropogenic methane emissions in Canada, as well as the policies addressing the management of those sources and the challenges to mitigating emissions from those sources.

Final remarks

- The research is in its early stages, and outcomes have not yet been produced.
- The expected outcomes of Victoria's work include a comprehensive overview of anthropogenic methane emissions in Canada, identification of gaps in policy coverage addressing these sources and a discussion of sector-specific challenges and opportunities for methane emissions policy and regulation.

Methane emissions policy and regulation in Canada: Assessing options and effectiveness

Maryam Lawal
LLM student

A comparison of the regulatory designs and approaches of the methane regulations of identified provinces as well as the federal government.

Introduction

Maryam Lawal's research will collect the methane regulations of the federal government and identified provinces — Alberta, Saskatchewan and British Columbia. It will examine the justifications provided by the federal government to grant federal equivalency for the identified regulations. It will also identify the components and compare the structures of each regulation while considering whether the varying regulatory designs may impair Canada's methane emissions reduction target. Various regulatory designs and theories will be studied to understand which regulatory design might be best for achieving real reductions in methane emissions.

Results

On Tuesday, May 12, 2020, Alberta released a revised version of its methane regulations. The strengthened amendments to the Alberta Energy Regulator Directives were made to stop the federal methane regulations from taking effect.

The Alberta methane regulations are less prescriptive about how companies meet their targets. The new methane regulation adopts a more flexible approach in comparison to the old methane regulation as companies are allowed to use averages instead of all facilities meeting emissions targets.

Final remarks

- In terms of the enforcement of the Alberta methane regulations, Maryam concludes that less prescriptive requirements adopted are more effectively monitored for compliance. She believes that it is easier to observe the flow rate of a piece of equipment as opposed to keeping track of a site-specific limit.
- Unlike a rule-based regulation, principle-based regulations are designed to set out general guiding principles that may or may not be industry-specific. On the efficacy of this regulatory design the regulation often states the legal standard that must be met and provides a legal test for the conduct that must be avoided.
- The use of smart regulations contemplates a combination of various effective regulatory instruments and coordination between governments. The benefit of this system allows for an improved standard of regulations and a crystal-clear depiction of how the government ought to perform its obligations under the regulations.
- On the use of the Best Available Technology (BAT), it was concluded that the BAT is much appreciated considering the amendments and modifications of laws to address changing circumstances. Hence, adopting the BAT renders it unnecessary "to continue to change the standard as new practices and technology become available".

DUVERNAY PILOT HYDRAULIC FRACTURE TEST SITE (HFTS)

Chris Clarkson, Kristopher Innanen, Roman Shor, Steven Bryant, David Eaton, Apostolos Kantzas, Bernhard Mayer

Background

Shell is implementing an Integrated Diagnostic Pilot in the Duvernay Shale (western Canada), which is analogous to the Hydraulic Fracture Test Site (HFTS) projects managed by Gas Technology Institute in the Permian Basin of the USA. A world-class dataset will be collected by Shell for the purpose of evaluating vertical and horizontal fracture geometry, extent of interwell communication ('frac hits'), stimulation effectiveness, improvement of petrophysical and geomechanical models, determination of cement isolation and fingerprinting of produced fluids to improve PVT models. The University of Calgary was invited to participate in the pilot. The pilot will be implemented from July to December 2020.

Research strategy

The University of Calgary, will work on five subprojects: (1) Post Fracture Pressure Decay (PFPD) led by Chris Clarkson, whose objective is to apply new models for evaluating pressure falloff data after the fracture stimulation treatment to evaluate variability in reservoir quality/ stimulation treatment results along the horizontal wells. (2) Advanced Passive Seismic Imaging using distributed acoustic sensing (DAS) led by David Eaton, whose objective is to apply advanced passive-seismic imaging methods to understand the dynamic interaction between hydraulic fracture stimulation and bedding plane/fracture fault systems. (3) Nano Particle Tracer Injection Field Trial led by Steve Bryant and Apostolos Kantzas, whose objective is to add nano particle tracers to at least two stages prior to flowback to determine which fractures are contributing to production. (4) Reservoir Geochemistry led by Bernhard Mayer, whose objective is to use core and cuttings collected in the vertical monitor well for a) chemical and isotopic characterization of H_2S found in the Duvernay and bounding zones and b) chemical characterization of dissolved solids in the Duvernay and bounding zones. (5) Machine Learning to Assist Real-Time Stimulation Decisions led by Kristopher Innanen, whose objective is to improve stimulation distribution effectiveness (SDE) in real-time through identification of and calibration based on complex data relationships between stimulation treatment pressure responses and other data, e.g., fibreoptic, seismic, etc.

Desired outcomes

- Project 1 will provide a stage-by-stage comparison of reservoir quality, fracture stimulation design and perforation cluster efficiency. The PFPD results will be integrated with surveillance results to demonstrate the use of PFPD for evaluating stimulation effectiveness in the absence of non-fibre equipped wells.
- Project 2 will produce a catalog of microseismicity, a reservoir-scale discrete fracture network model with estimated effective fracture conductivities and interpretation of aseismic slip using DAS to enhance reservoir characterization and risk analysis of casing deformation and induced seismicity.
- The results of project 3 will be used to interpret dominant frac contribution and will be integrated with field production and operations data such as pressure falloff analysis.
- Project 4 is expected to identify potential source(s) of H_2S and processes resulting in H_2S in production gas that can be used for mitigating H_2S risk. It will also be used to assess potential diffusion of hyper-saline water into the Duvernay Shale via natural fracture systems.
- Project 5 will deliver a tool for automation of stimulation decisions.

Duvernay pilot hydraulic fracture test site (HFTS)

Combining 3-D seismic with microseismic to derisk the Duvernay Formation

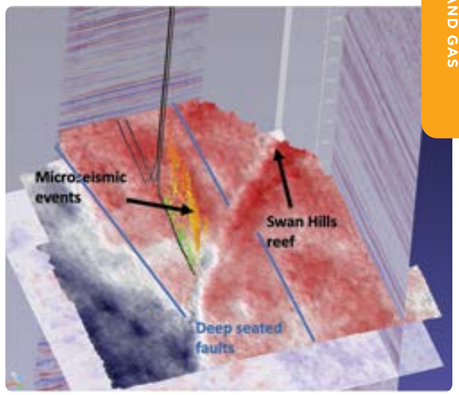
Ronald Weir
Postdoctoral Fellow

Introduction

Dr. Ronald Weir, PhD, aims to use reflection seismic and microseismic data to reduce risk associated with reservoir development in the Duvernay Formation unconventional hydrocarbon play.

Results

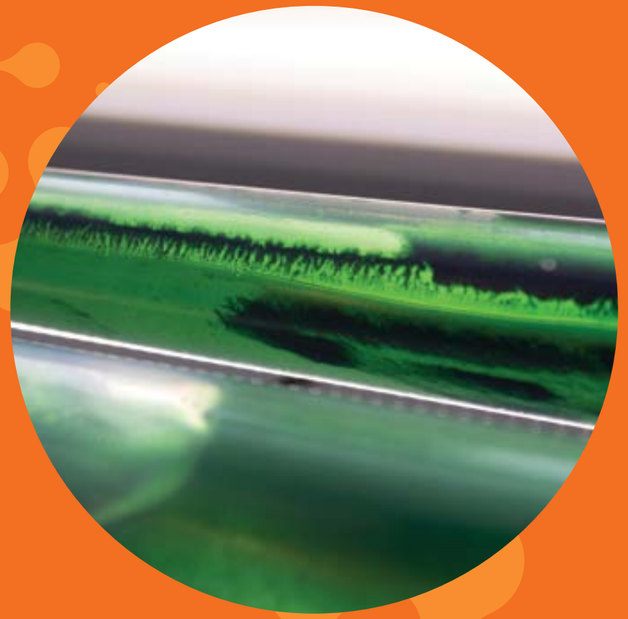
Ronald has developed an interpretive method using microseismic hypocenters and reflection seismic data to map faulting associated with deep-seated structures. These faults are used to predict the behaviour of induced fracture propagation and large (felt) induced seismic events. These results differ from previous models based on the assumption that the maximum horizontal stress axis dominates fracture propagation. Significant geologic features such as carbonate reefs in the Swan Hills formation also influence hydraulic fracture propagation. This interpretation uses the mapping of deep-seated basement flower structures, the associated strike-slip faults and the associated Riedel shear faulting.



Seismic depth map showing the Swan Hills Formation in a 3-D rendering, near Fox creek area of Alberta. The horizontal well bores are plotted in black, faults in blue, and an arrow highlights the Swan Hills reef

Final remarks

- Ronald has concluded that pre-existing faults dominate hydraulic fracture propagation in the Duvernay Formation hydraulic fracture treatment programs. This differs from previous reservoir modelling assumptions where the maximum horizonal stress is considered to dominate fracture propagation.
- Large (felt) induced seismic events are the result of reactivated basement faulting.
- Significant geological structures such as carbonate reefs exert an influence on hydraulic fracture propagation.



THEME 3: CO_2 CONVERSION

Theme 3 research, led by Dr. Marc Strous, PhD, is engaged in developing processes for CO_2 conversion and sequestration, as well as for converting waste biomass to fuels and products. One team converts CO_2 to fuel and commodity chemicals by combining recent advances in low-temperature and mixed-metal oxide catalysts with new, porous electrode materials for electrolytic cells. Other researchers convert CO_2 to biomass by combining designer microbiomes with printed electronics (organic solar cells). For CO_2 sequestration, they make use of the uniquely instrumented Alberta field site at the Containment and Monitoring Institute (CaMI). For carbon capture, Theme 3 researchers are developing new metal-organic frameworks and process configurations. This research envisages petroleum reservoirs as geological storage sites for CO_2, converting petroleum extraction from a net source of CO_2 into a net carbon-negative activity.

Prof. Marc Strous is the lead of this theme and Angela Kouris is the Research Associate. Other University of Calgary faculty members involved in the projects under Theme 3 are Profs. Anne Benneker, Joule Bergerson, Viola Birss, Steven Bryant, Hector De la Hoz Siegler, Michelle Dolgos, Ian Gates, Josephine Hill, Jianguang Hu, Kunal Karan, Md Golam Kibria, Steve Larter, Justin MacCallum, Nader Mahinpey, Sean McCoy, Warren Piers, Sathish Ponnurangam, Edward (Ted) Roberts, Roland Roesler, George Shimizu, Roman Shor, Samira Siahrostami, Marc Strous, Venkataraman Thangadurai, Jeffrey Van Humbeck and Gregory Welch.

PHOENIX (BIOMASS CONVERSION) – FORMERLY KNOWN AS SYZYGY

Jianguang Hu, Steve Larter, Jeffrey Van Humbeck, Venkataraman Thangadurai, Md Golam Kibria, Joule Bergerson, Sean McCoy

Background

Gradual shift from the traditional hydrocarbon-based “oil-refinery” to the sustainable carbohydrate-based “bio-refinery” could solve the raising energy and environmental issues. Biomass conversion into value-added chemicals and fuels provides a promising strategy to reduce the current pressure from global warming, environmental issues and the shortage of fossil fuel resources. This project focuses on multifunctional photo(electro) catalyst design for simultaneously producing gas fuels (hydrogen, methane, carbon monoxide, etc.) and value-added chemicals.

Research strategy

The objective of this project is to develop a clean technology platform “Photo-bio-refinery” that would enable valorization of various locally biomass wastes into high-value fuels and chemical feedstock to create alternatives to fossil fuel-based technologies. This project has significant potential for profitable collaboration with Canadian agricultural, pulping, biochemical and oil & gas industries, and the success of this project will contribute to making Canada a world leader in decarbonizing its economy. In this proposed biomass conversion platform, photo(electro)catalysts, substrate treatment and reaction condition all play important roles. For catalysts design, band-gap engineering, surface defect, heterojunction and hierarchically porous structure have been utilized to improve activity and endow the catalyst with unique selectivity for substrate conversion. For substrate conversion, bottom-up strategy (from basic unit of biomass building block components to large complex substrate) has been employed to simultaneously investigate mechanism and improve efficiency and selectivity. The final goal of this project is to directly utilize the plentiful raw biomass to selectively produce bio-chemicals along with high value gas fuels.

Desired outcomes

A minimum of ten academic publications every year are anticipated, as well as the obtainment of one to two patents at the end of the project. Additionally, this project will serve as a vehicle to establish strong collaboration with local biomass and energy related companies, and to gain the recognition of domestic and international research communities for biomass photorefinery.

Phoenix (biomass conversion) — formerly known as SYZYGY

Sulfide-based photocatalysts for sunlight driven lignin depolymerization

Bruna Goes Palma
MSc student

Introduction

Lignin is the second most abundant constituent of biomass and still has not been exploited to its fullest potential due to wide structural diversity, heterogeneity and stable chemical bonds. Conventional strategies to depolymerize lignin usually lead to nonselective bond-breaking due to the harsh conditions applied. Alternatively, photocatalysis has been valued as an ecologically benign alternative to induce the selective bond cleavage to functionalized aromatics under mild conditions. In her work, Bruna Goes Palma aims to present a route to directly depolymerize technical lignin under visible light on sulphide-based catalysts for the efficient production of valuable chemicals from this recalcitrant substrate.

Results

Bruna fabricated a series of Z-scheme cadmium sulphide-gold-bismuth vanadate (CdS-Au-$BiVO_4$) photocatalysts with morphology and constituent content regulated to achieve high lignin depolymerization efficiency. The gold (Au) nanoparticles present between cadmium sulphide (CdS) and bismuth vanadate ($BiVO_4$) acted as both electron transfer medium and photosensitizer. The scanning electron microscopy (SEM) results disclosed that the fabricated rod-like $BiVO_4$ is constructed by numerous nanoparticles, shown in Figure 1, and the X-ray diffraction (XRD) results, shown in Figure 2, revealed the presence of CdS in the composite and high crystallinity of CdS and $BiVO_4$. The photocatalytic activity of heterojunctions and solo photocatalysts were evaluated in the degradations of lignin model compounds under visible light irradiation. She observed only photocatalysts with a certain content of CdS presented activity in the cleavage of β-O-4 bonds of model compounds, but further studies are necessary to improve the reaction rate and conversion.

Figure 1

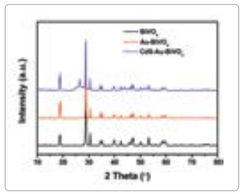


Figure 2

Final remarks

- Bruna concluded that thiol groups play an important role in the cleavage of β-O-4 bonds.
- Further studies are necessary to improve the photocatalytic performance. Additionally, it is also important to evaluate the ability of photocatalysts to break carbon-carbon bonds, which are very abundant in technical lignin.
- Her next steps are to compare the catalyst performance with transition metal disulfide photocatalysts and to test the best photocatalyst with technical lignin samples obtained from different extraction techniques.

Phoenix (biomass conversion) — formerly known as SYZYGY

Development of photo-electrochemical systems for energy storage via conversion of carbon dioxide, water and biomass to fuels and chemicals

Mohd Adnan Khan
Research Associate

Introduction

Mohd Adnan Khan is developing electrocatalytic systems for converting renewable energy to fuels and chemicals to achieve a higher grade of sustainability for the chemical industry. His goal is to develop novel catalysts and electrolyzer designs to selectively make valuable fuels and chemicals such as hydrogen, ethylene and carbon monoxide via electrochemical reduction of water and/or carbon dioxide. At the same time, he is investigating anodic water and biomass oxidation reactions for co-production of chemicals such as lactic acid, formic acid, gluconic acid (GNA) and glucaric acid (GRA). He is also working on a techno-economic and system-level analysis of such a process for large-scale industrial production.

Results

Mohd recently completed a study where he presented a detailed techno-economic analysis (TEA) of a potential photo-biorefinery approach for sunlight-driven electro-oxidation of glucose to produce valuable fuels and chemicals such as hydrogen, GNA and GRA. Under a base case scenario, the results are promising with a minimum selling price (MSP) of GRA at $6.94 per kilogram, which will be approximately 70 per cent lower than the current market price. The detailed breakdown and sensitivity analysis suggest that unlike conventional water electrolysis, the cost of raw materials and separation has a significant impact on the economics. Furthermore, they also establish performance targets for conversion (90 per cent), selectivity (90 per cent), feed concentration (0.5 moles per litre) and operating current density (0.4 amperes per square metre) such that if these targets are achieved, photo-electrochemical conversion of biomass to fuels and chemicals can become a very profitable option with MSP of GRA as low as $1.42 per kilogram.

Final remarks

- The study demonstrates how TEA can be used to establish catalyst performance targets such that if these targets are achieved, photo-electrochemical conversion of biomass to fuels and chemicals can become a very profitable option.

Phoenix (biomass conversion) — formerly known as SYZYGY

Solar driven selective conversion of glucose to value-added products

Ugochukwu Nwosu
MSc student

Introduction

The goal of this project is to develop and optimize a system by which glucose can be selectively converted to value-added products via photocatalysis. The main challenges associated with this are identifying a viable photocatalyst and optimizing the reaction conditions for selectivity. If successful, the project represents a sustainable alternative for valuable chemical production.

Results

Photocatalytic experiments show that glucose is readily converted by various catalysts in neutral and alkaline conditions. The mechanisms observed are oxidative in nature. In alkaline conditions, selective photocatalytic glucose conversion competes with the spontaneous conversion of glucose to lactic acid. So far, Ugochukwu Nwosu has been able to generate hydrogen from glucose using a functionalized carbon nitride catalyst. While this result is promising, the simultaneous production of glucose-derived molecules would enhance the value of the work. Future work will be focused in determining the mechanism of glucose oxidation as well as developing new photocatalysts capable of selectively oxidizing glucose.

Final remarks

- Synthesis of a cyanamide-functionalized carbon nitride photocatalyst has been achieved.
- Glucose can be oxidized to produce hydrogen using visible light.
- Ugochukwu is looking forward to developing new photocatalysts capable of simultaneous carboxylic acid production.

Phoenix (biomass conversion) — formerly known as SYZYGY

Jagos Radovic
Research Associate

Introduction

The goal of the Phoenix project is the production of low/zero CO_2 materials from bitumen fractions and biomass. Dr. Jagos Radovic, PhD, works on chemical fractionation and/or characterization of feedstocks (i.e., lignocellulose, asphaltenes) and products of their chemical and photo-catalyzed upgrading. He also collaborates on the development of chemical -omics process optimization tools through a combination of high-resolution mass spectrometry data and machine learning algorithms. Finally, he is one of the key technical contributors to the GRInstem-LysisLogic Inc. grant, developing high-risk, high-reward innovative technologies including advanced petroleum system tools, novel materials from petroleum industry by-products, climate change mitigation systems and chemical database intelligence for consumer products.

Results

Jagos developed workflows for fractionation and/or characterization of lignocellulosic and bitumen feedstocks and upgrading products using liquid chromatography, infrared spectroscopy and ultrahigh-resolution mass spectrometry. Bitumen fractions generated by Jagos were used by Dr. Jeffrey Van Humbeck, a faculty member from the chemistry department at the University of Calgary, to test chemical oxidation approaches for production of functionalized value-added materials. The promising potential of this experimental approach has been noticed by industry (Suncor) and the Alberta Innovates Bitumen Beyond Combustion (BBC) program, in particular for the production of carbon fibres. As a result, the research team, including Jagos, was awarded phase one funding in the BBC Carbon Fibre Grand Challenge. His main contributions to the GRInstem grant included development of methods for the extraction and analysis of wood compounds, for which relevance was validated by the industry representative, and technical assessment of ocean-based carbon capture technologies. This research has recently been presented at the international Goldschmidt virtual conference (June 2020). Jagos is also co-leading an innovation-focused initiative that will help the development of impactful ideas to commercial innovations.

Final remarks

- Bitumen fractions can be isolated and used as feedstock for chemical upgradation to value-added materials.
- Ultrahigh-resolution mass spectrometry is a suitable tool for detailed characterization of lignocellulosic biomass feedstocks and products.
- Initial methods have been developed for thermal and irradiation treatment of wood biomass, and the subsequent extraction and chemical analysis of compounds with commercial interest/value. Further method optimization based on the feedback from the industry representative is underway.
- Technical assessment of several ocean-based carbon sequestration technologies has been performed, and based on that report, proof-of-concept electrochemical experiments, in collaboration with the Thangadurai group, are planned for the next quarter.

Phoenix (biomass conversion) — formerly known as SYZYGY

Senthil Velan Venkatesan
Postdoctoral Fellow

Introduction

The project is aimed at developing technology for direct power production from oil and gas fields that leaves CO_2 underground. One of the options investigated involved an electron shuttle circulated into the reservoir to exploit the bioactivity for shuttle reduction. The reduced shuttle is then connected to processes linked to surface fuel cells, where the shuttle stays in a separate compartment. The initial idea had numerous variables to be considered across interdisciplinary areas such as bioactivity kinetics, reservoir with an optimal geometry, shuttle-pumping losses and bio-fouling of electrodes, but the research veered into the development of a novel energy storage/conversion device.

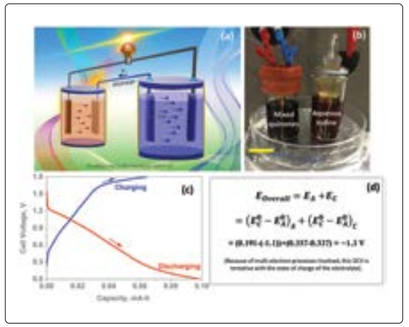


Figure 1

Results

Dr. Senthil Velan Venkatesan, PhD, has invented a novel membrane-free redox cell for energy storage. This design, shown in Figure 1a, unlocks a variety of opportunities for mass-transport independent energy storage technology.

The improved design features:

- Minimized self-discharge using aqueous electrolyte in the cathode chamber and non-aqueous electrolyte in the anode chamber, that eliminates ionomer coating on the auxiliary electrode.
- 100 per cent increase in coulombic efficiency at higher cycle numbers than its previous design.
- Metal-free energy storage using organic molecules and iodine with an improved open circuit potential of 1.4 volts and charge/discharge characteristics, shown in Figures 1b and c.
- Ni^{3+}/Ni^{2+} couple for alkaline condition, which owes many operational advantages such as minimized corrosion, etc.

Final remarks

- Senthil developed a new redox cell design for mass-transport independent energy storage towards low-carbon transition technologies.
- The non-combustion utilization route of bitumen is quite promising for a carbon-neutral future.
- The knowledge of electrode design is used in developing technologies for electrochemical reduction of CO_2.
- The research work resulted in a provisional patent application, four peer-reviewed international publications and presentations in six national/international events.

Phoenix (biomass conversion) — formerly known as SYZYGY

Sustainable energy & biomass photo-electro-reforming

Nael Yasri
Research Associate

Introduction

Using his background in electrochemistry Dr. Nael Yasri, PhD, aims to convert energy waste to value-added products. Part of his research is to develop new catalysts for carbon dioxide (CO_2) reduction and, at the same time, conversion of biomass waste to valuable products.

The electrochemical conversion of CO_2 is considered a promising strategy to enable the production of value-added energy carriers such as methylene, ethylene and carbon monoxide. Moreover, the replacement of fossil-based resources with those of sustainable and eco-friendly alternative resources motivates research to a unique notion of biomass conversion to fuel, which could provide environmental and economic benefits.

Results

Nael is developing catalysts that exhibit high production efficiencies for the electrochemical CO_2 reduction reaction in aqueous media using a conventional electrochemical flow design. In his prepared manuscript, a simple and facile electrochemical preparation method is demonstrated to assemble organometallic-based catalysts that can be employed for the electrocatalytic CO_2 reduction reactions to form carbon monoxide that can be switch to ethanol by switching the core metal in the metal-organic framework (MOF) structure.

Applying his electrochemistry background, Nael also prepared a set of electrode-modified catalysts that can be used for the selective electrochemical conversion of biomass waste to economically and industrially value-added products. This approach is ground-breaking in regard to waste conversion to value-added chemicals in an efficient manner.

Final remarks

- Nael concluded that MOFs are promising materials for efficient CO_2 reduction to value-added products.
- He believes that changing the morphology and the core metal can tune the type and the efficiency of the conversion processes.
- The next step is to stabilize the catalyst and to scale-up the process of CO_2 reduction.

Phoenix (biomass conversion) — formerly known as SYZYGY

Sunlight driven reforming of biomass for sustainable production of hydrogen and value-added products

Heng Zhao
Postdoctoral Fellow

Introduction

Dr. Heng Zhao, PhD, is focusing on setting up efficient systems for evaluating the photo(electro)catalytic conversion of biomass. He also works on fabricating suitable photocatalysts with hierarchically porous structures and high content of active sites, and on exploring the biomass photodegradation mechanism based on the experimental and theoretical calculation results. He already completed several photocatalyst designs and fabrications. These photocatalysts demonstrate good efficiency for biomass feedstock photoreforming for co-production of hydrogen and value-added chemicals.

Results

Heng helped complete the construction of a biomass photoreforming system, including several photo-reactor designs, and setting up standard photocatalytic processes and performance evaluation systems such as gas and liquid chromatography.

He successfully prepared several photocatalysts with multiple functions such as different morphologies of cadmium sulphide (CdS), a heterojunction based on $BiVO_4$, porous g-C_3N_4 with different co-catalysts, hierarchically porous TiO_2 and titanate perovskite, gold sol, silver sol and carbon quantum dots.

He completed the investigation of glucose and cellulose photorefinery by using a $Zn_{1-x}Cd_xS$ solid solution, 3DOM TiO_2-Au, and g-C_3N_4. The value-added products created with high efficiency were arabinose and lactic acid. His next steps are to try to use the photoreforming strategy to efficiently convert lignin and waste plastics to simultaneously produce gas fuels and value-added chemicals. He already submitted two research papers to scientific journals and is expecting to submit two more papers soon.

Final remarks

- Biomass photoreforming by proper photocatalyst design and reaction condition modification is feasible and promising to simultaneously produce gas fuels and value-added chemicals.
- This project is challenging in the following aspects: (1) how to efficiently convert biomass substrates under mild conditions; (2) how to improve the product selectivity; (3) how to create a relationship between photocatalytic principles and substrate conversion pathways.

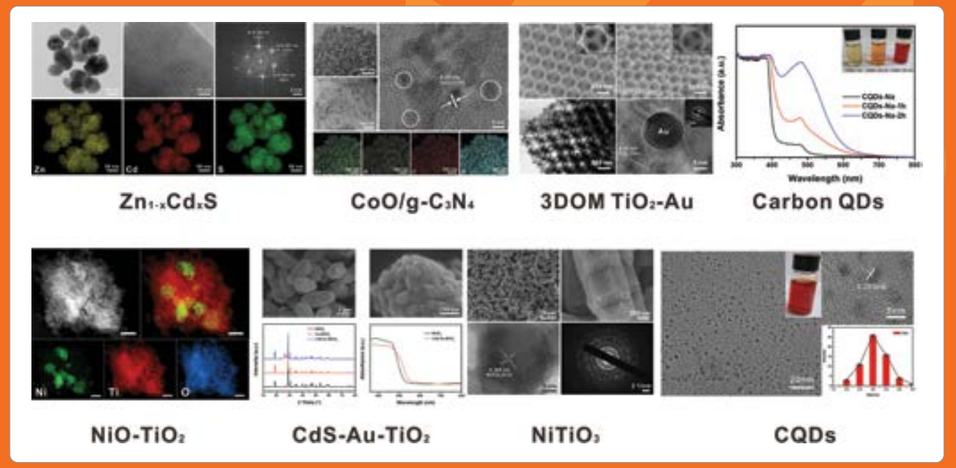


Figure 1

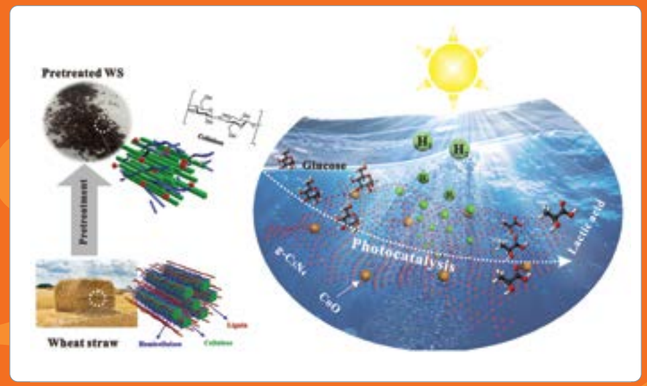


Figure 2

Figure 3

SYNTHETIC FUELS

Warren Piers, Roland Roesler, Gregory Welch, Kunal Karan, Viola Birss, Samira Siahrostami, Joule Bergerson

Background

Selective reduction of carbon dioxide to one product requires active, long lived catalysts that can be incorporated into continuously working devices. Among the possible products, CO is attractive because it can be converted to hydrocarbon fuels via known Fischer Tropsch technology. If the energy required to drive the catalytic CO_2 to CO conversion is achieved, carbon-neutral fuels — "Solar Fuels" — are possible.

Research strategy

A team of synthetic chemists, materials chemists, electrochemists and engineers are working on three fronts. New molecular electrocatalysts are being designed, prepared and tested. New methods for immobilizing catalysts on carbon-based materials for electrode modification are being developed to increase the stability and performance of the molecular electrocatalysts. These electrode materials are being incorporated into newly designed gas phase devices for continual production of CO from CO_2.

Desired outcomes

Excellent progress has been made on all three fronts. The team has developed methods for lowering the overpotential of existing and new catalyst designs. The ultimate goal is a "made in Calgary" molecular electrocatalyst. Three different immobilization techniques have been explored and one in which the catalyst is embedded in a polymer coating on colloid imprinted carbon or carbon nanotubes has proven to be the most effective. The research is exploring novel polymer structures to further enhance activity and longevity of the catalyst material. Finally, the gas phase device engineering had progressed and tests well using standard catalyst materials. The goal here is to incorporate their embedded catalysts into the device and evaluate its performance for this important process.

Synthetic fuels

Development of a new catalyst for CO_2 electroreduction reaction

Amir Alihosseinzadeh
PhD student

Introduction

The carbon dioxide electroreduction reaction (CO_2RR) has attracted great attention because of its potential to convert CO_2 to more value-added products such as syngas and hydrocarbons. In this project, Amir Alihosseinzadeh's focus is on the development of a highly efficient and stable novel catalyst for CO_2RR with a high selectivity towards formation of CO, hydrocarbons and multi-carbon oxygenates. Among different types of catalysts which have been studied for CO_2 reduction, transition metals like silver exhibit a high selectivity towards formation of CO at low overpotential and high efficiencies. Also, polymer-based catalysts, such as polydopamine, have demonstrated a high surface area, low cost and robust characteristics with significant electroactivity for CO_2RR application.

Results

The project can be classified into a number of categories. In the cata-test setup, a gas-phase electrolyzer device has been designed to evaluate the catalytic performance of catalysts. In terms of product analysis, an online/offline gas chromatographer (GC) was designed and calibrated for the analysis of the products. The configuration of the GC is set to analyze the potential carbon-contained products of CO_2RR (H_2, CO_2, CO, CH_4, C_2H_4, C_2H_6, ... up to C_4 compounds). A protocol was developed for electrochemical characterization of catalysts in the device. A silver (Ag) nanoparticle-based electrode was fabricated and analyzed on the CO_2RR device as the benchmark catalyst, and different types of cation and anion exchange ionomers/membranes are studied. The Ag benchmark electrode shows more than 90 per cent selectivity for CO production using anion exchange membrane/ionomer as the solid electrolyte. Different types of catalysts (such as transition metal- and rare earth-based components) and substrates (like carbon-based and polymer-based materials) are synthesized, and their performance on CO_2RR is under investigation. The performance of iron-based (FeTPP) and cobalt-based (CoPc) molecular catalysts in the gas-phase CO_2 electrolyzer is studied, along with the effect of the catalyst loading and the long-term stability of the catalysts. Lastly, the structural and electrochemical characteristics of the prepared catalysts/electrodes are characterized based on atomic force microscopy (AFM), X-ray powder diffraction (XRD), Brunauer–Emmett–Teller (BET), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDS), cyclic voltammetry (CV), linear sweep voltammetry, (LSV) and electrochemical impedance spectroscopy (EIS).

Final remarks

- A functional gas-fed electrochemical reactor, equipped with an online GC analyzer, was developed.
- A silver nanoparticle-based benchmark electrode was fabricated, with around 150 milliamperes per square centimetre current density, 90 per cent CO selectivity, and more than 100 hour stability. However, another order of magnitude improvement in long-term stability is needed to attract commercial interest.
- Amir is working on the development of new catalysts and electrode structures to improve the activity, selectivity and stability of the catalyst. To do so, an in-house metal-polymer promoted electrode is being synthesized and is under investigation.
- Syngas and CO are the main products of the reaction; however, some desirable products such as lower hydrocarbons (CH_4, and C_2H_2) are obtained by optimizing the reaction and electrode parameters.

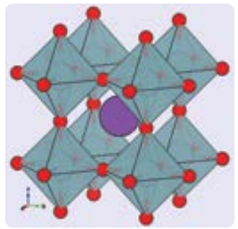
Synthetic fuels

Data-driven search for perovskites as electrochemical CO_2 reduction catalyst

Claude Coppex
PhD student

Introduction

Claude Coppex is performing density functional theory (DFT) high-throughput computations to find suitable catalysts for photocatalytic CO_2 reduction. This specific computational approach has been developed within the last 20 years and agrees well with experimental measured overpotential. While predictions for metal catalysts are already being generated with high-throughput calculations, perovskites are sparsely investigated. Compared to common metal alloy surfaces, they offer a completely different surface structure, geometrically and electronically. The many intermediates which can be obtained with CO_2 reduction and coverage of the surface with hydroxy groups and/or hydrides offer a complex reaction network.



Results

Claude found 22 cubic theoretically stable perovskites under operating conditions (pH=14, U=-0.84). Some of those have already drawn the interest of experimentalists and/or have been mentioned by other data-driven studies. He investigated the minimum energy pathway for CO_2 reduction to CH_4 for six of them known to be catalytically active surfaces, (Ca, Sr, Ba)TiO_3 and (K, Na, Tl)TaO_3. He also investigated the hydrogen and oxygen coverage of those perovskites under operating conditions, which revealed the importance of including those perspectives, as tantalum (Ta) perovskites show a significant hydroxode (OH) coverage during operation, influencing the electronic structure.

Final remarks

- While a low oxygen coverage for (Ca, Sr, Ba)TiO_3 and a mechanism to methane over formic acid was found. (K, Na, Tl)TaO_3 calculations imply a higher oxygen coverage.
- The reduction pathway on titanates shows a high selectivity to methane.

Synthetic fuels

Novel homogeneous electrocatalysts for CO_2 reduction

Zack Dubrawski
PhD student

Introduction

Recent literature suggests design principles for molecular CO_2 reduction electrocatalysts. By applying these principles, Zack Dubrawski and the synthetic team are rationally developing novel organometallic molecules that can reduce CO_2 to industrially useful one carbon (C-1) products with selective and efficient catalysis. The synthesis of these molecules can be challenging and there is no guarantee that they will be catalytically active once synthesized. However, the impact that these compounds will make will be far-reaching as novel CO_2 reduction electrocatalysts may be the key to large-scale CO_2 abatement.

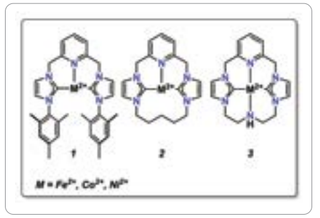


Figure 1

Results

Following up on the successes of the 1,3,5-triazapentadienyl-2,4-bis(2-pyridyl) (TAPPy) platform (Sustainable Energy & Fuels, 2019, 3, 1172-1181), Zack has since been developing a family of carbon-nitrogen-carbon (CNC) pincer complexes aimed at stabilizing reactive intermediates through the CO_2 reduction catalytic cycle, depicted in Figure 1. Going from complex 1 to complex 3, Zack and his team can systematically alter the binding motif of the ligand and thus skew reactivity to more competent catalysis. Specifically, complex 3 has a protic amine adjacent to the reactive metal centre. It is anticipated that this amine will stabilize the highly reactive CO_2 adduct of the complex through hydrogen bonding. By lowering the thermodynamic barrier to these intermediates, Zack can reduce the overall energetic requirements for catalysis.

Final remarks

- The ligand synthesis has been developed and metalation proceeds smoothly.
- Preliminary results are inconclusive but the project is ongoing.

Synthetic fuels

Polydentate ligand design for electrocatatlytic CO_2 reduction

Alexander Harrison
MSc student

Introduction

Alexander Harrison works with a multidisciplinary team targeting the conversion of carbon dioxide (CO_2) to value-added products such as carbon monoxide (CO), formate (HCOO-), and carbonate ion (CO_3^{2-}). His research focuses on developing novel electrode-supported catalysts employing earth-abundant transition metals for the electrochemical reduction of CO_2, and tailored towards high efficiency and selectivity. The design has a substantial impact on the affinity and selectivity for CO_2 reduction, where the electronic and steric properties of the catalytically active site need to be carefully tuned for high faradaic efficiencies, stability and low overpotentials.

Results

Throughout the first year of his graduate degree, Alexander has worked closely with graduate students in the groups under Profs. Roland Roesler, Warren Piers and Gregory Welch towards the development of catalysts for the electrochemical reduction of CO_2. An extensive review of the literature has led him to the targeted synthesis of a novel modification to the existing 2,2'-bipyridyl ligands. The incorporation of N-heterocyclic carbenes (NHCs) into the 2,2'-bipyridyl framework enhances the subsequent catalyst stability and reduces the ligands reduction potential. Promising results from the rhenium complex of the aforementioned ligand have emerged from preliminary electrochemical testing. The products of the electrochemical reduction of CO_2 with this complex are unprecedented for these rhenium-bipyridyl systems. Alexander believes that ascertaining the mechanism of this reactivity will be impactful to the field as it would provide valuable tools for ligand tuning with the purpose of modifying catalyst selectivity.

Final remarks

- Alexander has synthesized a rhenium-bipyridyl catalyst for the electrochemical reduction of CO_2.
- His findings suggest that this new rhenium complex reduces CO_2 by a currently unknown mechanism that is uncommon to these systems.
- He is currently investigating the mechanism of reactivity and identifying the products of the catalysis.

Synthetic fuels

New materials for conversion of CO_2 to value-added products

Josh Koenig
PhD student

Introduction

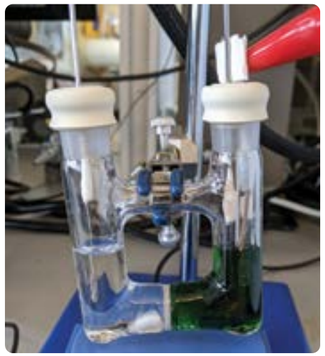
The link between increased atmospheric CO_2 levels and climate change has inspired a variety of emission mitigation efforts, including the electrochemical conversion of CO_2 to value-added chemicals. The major challenge facing the wide-scale implementation of these technologies is the high energy input required to activate CO_2. Josh Koenig's goal is to develop the next generation of catalysts that facilitate the efficient and selective CO_2 conversion, all while using the lowest energy input. Josh's current research strategy focuses on linking organic chromophores to champion CO_2 electrocatalysts with the intent of improving catalyst durability, while also reducing the energy input of the system.

Results

Perylene diimide (PDI) is a photosensitizer and is well-recognized for its high absorptivity, redox stability and synthetic versatility. Despite these favourable properties, no CO_2 conversion catalysts containing PDI have been reported in the literature. By tethering this PDI unit to a current state-of-the-art CO_2 electrocatalyst, Josh has discovered that PDI:

- Serves as an electron reservoir for the electrocatalyst, thereby lowering the electrical energy input;
- Enables electrode immobilization, potentially facilitating the implementation of PDI-tethered electrocatalysts in large-scale electrolyzers;
- Performs CO_2 conversion photocatalytically, opening up the possibility of using solar irradiation rather than electrical energy.

Josh and the research team are currently preparing a manuscript to detail their findings, as they believe that these discoveries could have great significance on the future design of novel CO_2 electron and photocatalysts.



Final remarks

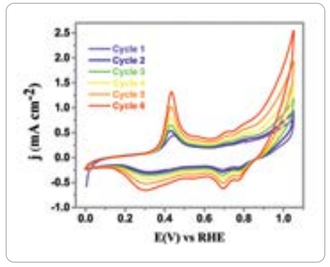
- They have developed a new class of CO_2 electro- and photocatalysts whose rich chemistry allow for material properties to be tailored to further improve catalyst performance.
- Their ongoing research efforts are focused on the development of design principles for these PDI-tethered electrocatalyst systems.
- This research helped earn Josh an NSERC Canada Graduate Scholarships — Doctoral.

Synthetic fuels

Manila Ozhukil Valappil
Postdoctoral Fellow

Introduction

Energy production secures the first place among humanity's top ten challenges for the next 50 years. Simultaneously, the rise of CO_2 levels in the atmosphere poses a major threat to the world's climate. Through this project, Dr. Manila Ozhukil Valappil, PhD, aims to achieve lower carbon emissions while simultaneously producing energy. Her research goal is the synthesis and electrochemical evaluation of mesoporous (tunable pore size 5-100 nanometres) freestanding carbon film-supported molecular organometallic CO_2 electroreduction (CO_2RR) catalysts for selective reduction to carbon monoxide (CO). Molecular catalysts can be tethered to carbon electrodes by electrochemical coupling reactions. The wettability of carbon supports can be customized via surface functionalization and it is easy to scale up.



Results

In collaboration with other Canada First Research Excellence Fund (CFREF) team members, Manila has started exploring molecular organometallic electrocatalysts (MOCs) and their anchoring to high surface area nanoporous carbon electrodes. Along with conducting a literature review, she has been actively involved in discussions related to various MOCs and various routes for their anchoring to carbon supports. As a preliminary step, she learned to synthesize porous carbons, colloid imprinted carbons (CICs) and a nanoporous carbon scaffold (NCS), and studied their electrochemical properties. Her current focus is on understanding electropolymerization for anchoring moieties such as aniline and pyrrole of a re-bipyridine-based MOC on nanoporous carbons, a key step in this project. Optimization studies with appropriate electropolymerization conditions will be carried out to identify the best performing CO_2RR catalyst. She is also interested in exploring the oxidation of the CIC and NCS for use as an anode in a CO_2 electrolyzer.

Final remarks

- MOCs based on rhenium bipyridine anchored onto porous carbon supports will be explored to determine their CO_2RR catalytic performance.
- The studies involve various strategies for anchoring MOCs using a range of covalent binding routes such as oxidative polymerization, diazonium chemistry, vinyl attachment, etc. However, the key challenges are to determine active surface coverage, maximize coverage and achieve stability.
- Oxidative polymerization to form polyaniline, polypyrrole, etc., has been explored, starting from basic studies with a glassy carbon electrode to the CICs and then NCS. The main goal is to obtain a conformal coating of the polymer with controllable thickness on porous carbons.
- The CICs and NCS are also being explored for use as an anode in a CO_2 splitting cell, also determining their propensity for oxidation-induced degradation.

Synthetic fuels

Electrocatalysts for CO_2 reduction based on mesoionic carbenes

Thorsten Scherpf
Postdoctoral Fellow

Introduction

To be economically viable for large-scale industrial applications, an electrocatalyst must be inexpensive to produce and have a long life under the conditions of catalysis. Mesoionic carbenes are a class of strong donor ligands which form an especially robust carbon-metal bond that is highly stable even in harsh environments, like those present during the electrochemical reduction of CO_2. Additionally, these ligands are easy to synthesize, through well-established copper-catalyzed "click" reactions. These aspects make them very promising electrocatalysts for the production of renewable fuels.

Results

Dr. Thorsten Scherpf, PhD, has begun to synthesize a diverse set of multidentate ligands, using the copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC) and subsequent arylation reactions to produce molecules incorporating one or more 1,2,3-triazolium moieties. The structure of the ligands was chosen to cover several different ligand geometries to study the influence of the binding mode of the ligand towards electrocatalysis. Transition metals will then be incorporated into these ligands to produce the final catalysts, which will be tested for their ability to perform CO_2 reduction. Here, a special focus will be the first-row transition metals since they are more abundant and cheaper. Depending on these results the structure of the ligands will be modified to improve the performance of the electrocatalysts.

Final remarks

- Thorsten is synthesizing a series of new transition metal complexes based on mesoionic carbenes.
- These ligands are very promising as highly stable CO_2 reduction catalysts.
- After assessing their ability in the CO_2 reduction, he will optimize their structure to produce more active catalysts.

Synthetic fuels

Structural evolution in photodeposited nickel (oxy)hydroxide oxygen evolution electrocatalysts

Martin Schon
Guest Postdoctoral Scholar

Introduction

Compared to their crystalline counterparts, amorphous metal oxides significantly expand the range of material parameters. However, predictions of the exact nature of the amorphous phase and its effect on material properties are still elusive. Thorough structure-property investigations of well-known model systems are thus necessary before predictive control of useful material properties is obtained. In this work, Dr. Martin Schon, PhD, fabricates a series of photo-deposited nickel (oxy)hydroxide (generally denoted as NiOx) thin films and anneal them at temperatures up to 1000 C. Extended X-ray absorption fine structure (EXAFS), X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) are used to determine the local structure, allowing them to correlate to measured electrochemical properties.

Results

In the research tests, Martin found an amorphous nickel hydroxide $Ni(OH)_2$-like local structure for annealing conducted below 250 C followed by an amorphous-to-amorphous phase transition to a nickel oxide NiO-like structure by 300 C. This provides evidence for different amorphous polymorphs in this NiOx system. Figure 1 depicts that above 400 C a cubic NiO XRD diffraction pattern is detected. Electrochemically, Martin found a stepwise increase of the onset overpotential at this transition, indicating a change in the potential-determining step and possibly the oxygen evolution reaction (OER) mechanism. The Tafel slope decreases linearly with annealing temperature, which they attribute to a decrease in (Ni)OOH reaction intermediary adsorption, supported by the in-operando ultraviolet-visible (UV-Vis) electrochromism, shown in Figure 2. Furthermore, they found a nickel oxyhydroxide NiOOH coordination after catalytic activity that was increasingly strained with annealing temperature, which manifested in higher electrochromic colouring rates and thus lower adsorption energies. Martin identified this as the root cause of the lowered intermediary adsorption. Thus, nanocrystalline NiO should kinetically be a superior catalyst to amorphous $Ni(OH)_2$. However, at their benchmarking value of 10 milliamperes per square centimetre the amorphous material exhibited lower overpotential, due to a combination of lower onset potential, large chemically active surface area and mass transport limitations under the applied conditions.

Final remarks

- Martin's research provided evidence for polyamorphism in the NiOx material system.
- Martin presented an original method to measure reaction intermediary coverage and its effect on the catalytic efficiency, as measured by the Tafel slope.
- The research determined strain as the root cause for changes in reaction intermediary coverage.
- The research provided a method to optimize future catalyst design.

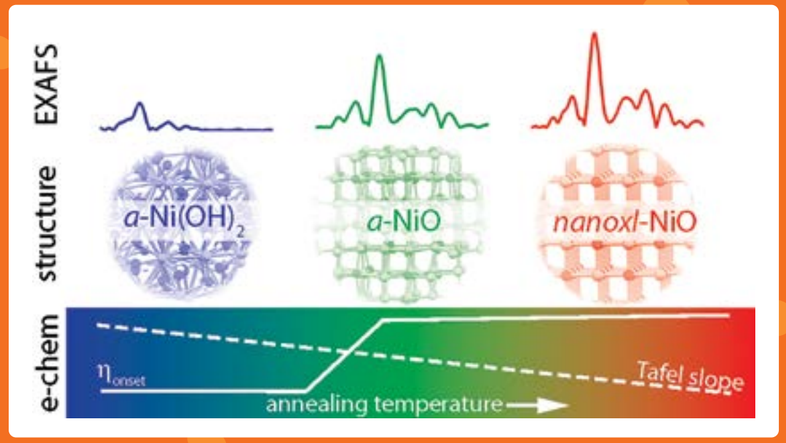


Figure 1

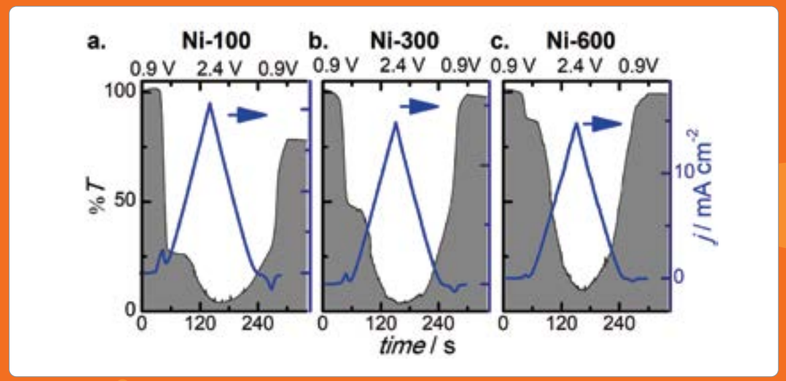


Figure 2

Synthetic fuels

Development of electrodes for CO_2 electrolyzer and its electrochemical testing

Anusree Unnikrishnan
Postdoctoral Fellow

Introduction

Since excessive levels of CO_2 contribute to global warming and drastic climatic changes, today's energy and environmental research is aimed towards developing cutting-edge technologies for CO_2 capture, conversion and utilization. One approach to solve this problem is the electrochemical conversion of the CO_2 gas into value-added fuels which can also supplement the alternative energy reserves. One of the main objectives of the research of Dr. Anusree Unnikrishnan, PhD, is to development electrodes which can be used for the efficient electrocatalytic reduction of CO_2. She also aims to increase the performance, product selectivity and system durability of the developed electrochemical system.

Results

Anusree's research is still in an infant stage as the global pandemic greatly hampered her research activities. The focus of her research is to optimize the complex multi-material structure of the CO_2 electrodes for gas-fed CO_2 electrolysis. She has completed the literature review and initiated the first trial runs of experiments. Her next steps will be to focus on optimizing the CO_2 electrode through the systematic study of the effect of various electrode parameters including ionomer content, catalyst loading and catalyst nanoparticle size. The aim of her work is to modify the electrode design to increase the electrocatalyst utilization and reduce the mass transfer limitations.

Synthetic fuels

Development of molecular catalyst-based hybrid systems for electrocatalytic CO_2 reduction

Janina Willkomm
Postdoctoral Fellow

Introduction

Dr. Janina Willkomm, PhD, aims to assemble a hybrid system for electrochemical CO_2 conversion based on molecular catalysts bound to nanostructured carbon supports (Figure 1A). Creating a stable and efficient hybrid electrode that also operates under environmentally-friendly conditions (i.e., pH neutral aqueous buffer) remains one of the major challenges in the field. Janina aims to explore various tethering strategies to overcome the issue of instability. Using nanostructured carbon supports that provide large surface area further helps her to achieve high catalyst loadings, and ultimately results in a better performance of such a molecular catalyst-hybrid device.

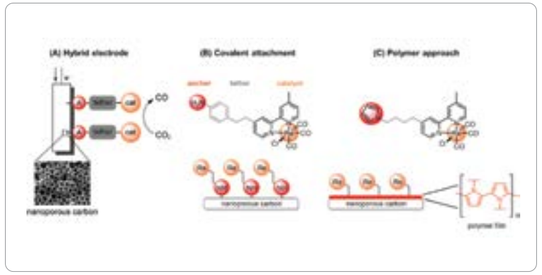


Figure 1

Results

Figure 1A illustrates Janina's investigation of the tethering of a well-studied rhenium-based molecular CO_2 reduction catalyst to the nanoporous carbon surface where the catalyst was modified with different anchoring moieties. Figure 1B exemplifies the achieved attachment of the rhenium-based catalyst via a covalent carbon-nitrogen bond, nonetheless, this first hybrid system rapidly degraded when tested under catalytic CO_2 conversion conditions. Figure 1C and Figure 2A show the significantly improved stability that Janina was able to attain by using a polymer approach where the rhenium complex is incorporated by a poly-pyrrole film that is directly formed on the carbon material. Further, she succeeded in the application of this second-generation hybrid electrode in aqueous media. Figure 2B depicts that CO_2 was continuously converted into CO with high efficiencies (greater than 90 per cent) over the course of a six-hour experiment.

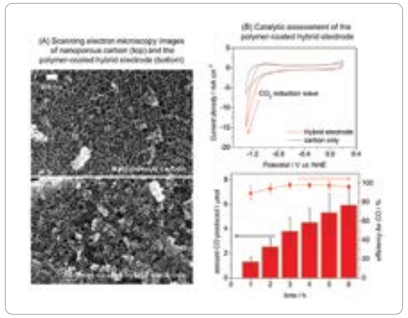


Figure 2

Final remarks

- Moving from a direct anchoring strategy (i.e., a direct covalent bond between catalyst and material surface) to a polymer approach has allowed Janina to develop a hybrid electrode for catalytic CO_2-to-CO conversion in water.
- Other monomers will be explored as polymerizable anchoring groups to optimize the properties and stability of the rhenium catalyst polymer layer.
- In collaboration with the Birss group, her next step is the up-scale of her polymer system from a batch to a flow-type device.

BIOENERGY

Marc Strous, Jinguang Hu, Gregory Welch, Jeffrey Van Humbeck, Samira Siahrostami, Justin MacCallum, Hector de la Hoz Siegler, Josephine Hill, Sathish Ponnurangam, Joule Bergerson

Background

In the next ten years, adoption of renewable energy and electrification of transportation, will contribute to reducing carbon dioxide emissions. However, the pace of change will likely be too slow to meet global targets for "safe" carbon dioxide concentrations in the atmosphere. Thus, industry will eventually depend on development of technology that can actually remove carbon dioxide from the air, compensating for past emissions.

Research strategy

This research takes on the ultimate challenge of realizing a technology that captures CO_2 from the air, while producing energy and revenue. The technology harnesses the power of alkaline Soda Lakes, natural ecosystems that have sequestered carbon dioxide from the atmosphere on a massive scale in Earth's geological past. This research integrates this biotechnology with organic solar cells, roll-to-roll manufacturing and machine learning to reduce costs and environmental footprint and produce a portfolio of useful and valuable products.

Desired outcomes

This research aims to achieve the commercialization of biotechnology converting CO_2 from the air into a valuable product while producing energy and the commercialization of organic solar cells based on green chemistry.

Bioenergy

Modification of cellulose biomaterials with carbohydrate binding modules

Brett Abraham
MSc student

Introduction

Brett Abraham's project involves the generation of cellulose-based biomaterials modified with recombinant carbohydrate binding modules (CBMs) for different biochemical and biomedical applications. Cellulose is a natural and renewable biomaterial, and CBMs are peptides with specific binding affinity towards different types of cellulose. Using synthetic biology, recombinant proteins can be produced that link CBMs to other bioactive enzymes. This allows for these fusion enzymes to be immobilized on different cellulose materials. Brett aims to use CBMs in different applications such as in the biodesulferization of petroleum distillates and the degradation of plastics, as well as other biomedical applications.

Results

Brett has generated several different materials out of cellulose biomass. On a macroscopic scale, these materials include two-dimensional sheets, hollow tube/fibres and spheres of bacterial cellulose. On the microscopic scale, he has also generated microspheres of carboxymethyl cellulose and microcrystalline cellulose for applications in bioreactors. These microspheres will be used along with CBM-fusion enzymes, immobilizing these catalytic enzymes on these suspended beads allowing for the enzymes to be recovered and recycled. Brett has also developed synthetic plasmids expressing different CBM and enzyme combinations. Preliminary enzyme production and purification show promising results and enzyme validation will follow soon.

Final remarks

- Brett has generated cellulose microspheres for applications in bioreactors. The next step is to modify these microspheres with CBM-fusion proteins towards different outcomes.
- He has also produced several plasmids for the production of different bioactive proteins and enzymes. The next step is to produce these enzymes efficiently and validate their catalytic ability.
- His future aims are to use these biomaterial-enzyme constructs in the biodesulferization of petroleum distillates, the degradation of plastics and other biomedical applications.

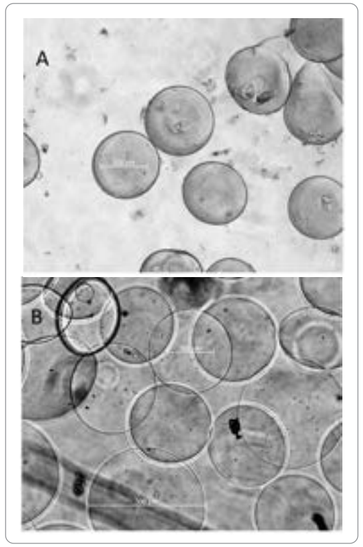


Figure 1. Microspheres generated from (A) carboxymethyl cellulose and (B) microcrystalline cellulose.

Bioenergy

Alireza Aslani
Postdoctoral Fellow

Introduction

Dr. Alireza Aslani, PhD, works on techno-economic and life cycle assessment of multi-product bioenergy, including CO_2 conversion. He assesses the costs and environmental impacts of bioenergy technology to aid technology developers to evaluate combinations of technologies and create process improvements. In this project, he assessed technology that cultivates algae using sunlight and CO_2 to produce renewable electricity through the generation of solar cells, pure oxygen, phycocyanin and renewable methane.

Results

Alireza has developed a techno-economic analysis (TEA) of the Bioenergy-Excel Tool. It is a user-friendly tool that can be adjusted to different scenarios and scale-ups. The analysis shows that 1.3 kilograms of captured CO_2 per kilogram of cultivated algae can be achieved in the Calgary climate area. Also, the generated electricity can support the required electricity for the system. Therefore, not only is this technology a carbon mitigation process, but it can also produce valuable products to offset the costs of the system including phycocyanin, electricity and methane. Alireza has also developed a new framework to identify the system's problems and develop innovations.

Final remarks

- At the commercial scale and per hectare of algae cultivation, the exported electricity to the grid can support over 320 detached houses in Alberta and the exported methane can support 65.
- At the commercial scale, the process could be competitive with other CO_2 conversion technologies in terms of cost parameters (e.g., direct air capture).

Bioenergy

Integrated large area organic photovoltaics into a photobioreactor

Edward Cieplechowicz
PhD student

Introduction

The overall goal of the team is to create a clean energy photobioreactor capable of reducing CO_2 emissions and generating high value-added products. Organic photovoltaics (OPV) have been identified as a perfect matching technology due to their flexibility to adapt on a variety of form factors of the photobioreactor. The colour tunability of OPVs allows for the selective transmission of photons to the bioreactor, while non-transmitted light is converted into electricity. The project goals are to develop large-area semi-transparent OPVs, acting as both light filters and converters to lead to a self-powered photobioreactor.

Results

Edward Cieplechowicz's role within this project has been to develop new photoactive materials and establish large area printing conditions. To date Edward has demonstrated the efficient synthesis of champion photoactive materials on scales appropriate for photovoltaic module fabrication. He has helped demonstrate the viability of slot-die fabricated OPV devices and optimized printing conditions to deliver large-area photoactive films, fully laminated with the addition of UV filters, for use as optical filters on the bioreactors. Edward has successfully synthesized a library of perylene diimide pi-conjugated small molecules for the development of a large-area semi-transparent OPV for the photobioreactor. Next steps are to design and synthesize pi-conjugated materials that facilitate greater charge transport to further improve OPV performance, while retaining solution processability from green solvents to streamline OPV module fabrication.

Final remarks

- Edward demonstrated a streamlined procedure for delivering flexible, coloured optical filters for use on the photobioreactors.
- He successfully designed and synthesized a library of perylene diimide pi-conjugated small molecules that are solution-processable in non-halogenated solvents for large area OPVs.

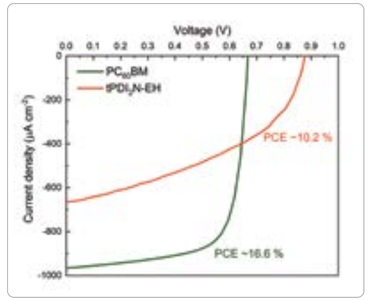
Bioenergy

Indoor organic photovolataics (IPVs) by slot-die coating methods

Sergey Dayneko
Postdoctoral Fellow

Introduction

The overall goal of Dr. Sergey Dayneko, PhD, and his research team is to develop indoor organic photovoltaics (IPVs) by slot-die coating methods. The perylene diimide (PDI) dyes have been identified as a perfect material for IPVs due to strong visible light absorption and excellent electron-accepting and transporting abilities. The project thus involves the development of IPVs which can deliver electrical power to wireless electronics such as smart housing sensors and sensors for the Internet of things (IoT).



Results

To achieve the project goal, Sergey and his team use a complimentary approach involving material design and preparation, performance simulation under different indoor source, and small-scale performance optimization of the IPVs and large-scale IPV coating. In the past year, he developed four different types of IPVs based on various materials to efficiently accumulate energy from cold to warm indoor light sources. He has been optimizing the bulk heterojunction layer using slot-die coating methods, which opens a way to make large-area IPV devices. The best IPV devices made by slot-die coating methods have produced power conversion efficiency (PCE) up to approximately 16 per cent, which is enough to power the smart housing sensors and sensors for IoT over a few months and even years. Sergey has also been collaborating with Brilliant Matters to achieve the objectives of this project. The results of this project have been published in *ACS Applied Materials & Interfaces*.

Final remarks

- Sergey has completed the project and has delivered high performance IPVs.
- He has established a streamlined procedure to slot-die printing of large-area photovoltaic devices.
- He is currently transferring his skills to print large-scale flexible organic light emitting diodes (OLEDs) and quantum dot LEDs (QLEDs).

Bioenergy

Downstream processing of algal biomass

Cigdem Demirkaya
PhD student

Introduction

Sustainability is a key factor in the development and application of biofuel production from microalgae, a promising alternative to non-renewable energy sources. Biogas production from organic materials by anaerobic digestion is a natural and efficient way of turning complex organic matter into a fuel (i.e., methane) that is fully compatible with our existing energy infrastructure. A combined approach to the production of biogas and bioproducts from microalgae is the basis for a sustainable biomass conversion process. Cigdem Demirkaya's research project entails the production of clean, low carbon and economically feasible biogas and high value-added bioproducts by anaerobic digestion of algae. To achieve her goal, Cigdem proposed a two-phase anaerobic digestion process consisting of a dark fermentation step where hydrogen, volatile fatty acids and valuable pigments are produced, followed by methanogenesis in a second step.

Results

Cigdem has performed the dark autofermentation of algae in batch mode. The organic carbon content in the biomass is converted to volatile fatty acids and hydrogen by the autofermentation ability of algae. Results from these experiments have shown that there are several high value-added bioproducts that can be obtained from the different stages of anaerobic digestion while producing methane (CH_4). In addition, she has performed batch anaerobic digestion experiments of autofermented and fresh microalgal biomass with different methanogenic inoculum sources. Her study demonstrated that it is feasible to overcome the challenges introduced by the highly alkaline and pH microalgal cultivation system such as ammonia inhibition and CH_4 production. With the results obtained from both batch dark autofermentation and anaerobic digestion, a continuous integrated autofermentation and CH_4 production process is currently being developed.

Final remarks

- This project will lead to the development of an economically feasible process for the production of bioenergy and valuable bioproducts from CO_2 and sunlight.
- The autofermentation demonstrated that there are many potential high value-added products that can be recovered to improve the economic viability and the sustainability of the process.
- The biofuel produced will further add to the knowledge of anaerobic digestion and how to control carbon partitioning between the different stages of the process to produce biogas and high value-added products at the same time.

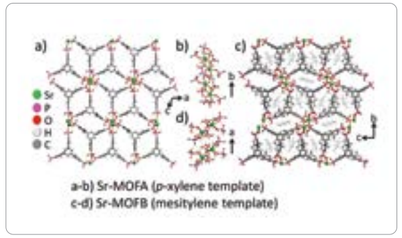
Bioenergy

Self-assembling porous metal-phosphonate frameworks

Martin Glavinovic
PhD student

Introduction

The success of carbon capture and sequestration hinges on the improvement of the carbon dioxide (CO_2) capture phase. Martin Glavinovic's project involves the design and synthesis of robust microporous materials that selectively adsorb CO_2 from the highly acidic and humid mixtures typical of fossil fuel flue gas. The materials under study are metal-organic frameworks (MOFs): porous crystalline molecular networks composed of metal ions and organic linkers. Martin's research focusses on the use of phosphonate linkers. Although they are both difficult to synthesize and to use, phosphonate linkers have significant potential in yielding extremely robust solids.



a-b) Sr-MOFA (*p*-xylene template)
c-d) Sr-MOFB (mesitylene template)

Results

Owing to their ability to connect to metals in a variety of ways, controlling the self-assembly of phosphonate linkers has been a major challenge. Due to their flexibility, they often self-assemble as layered networks with minimal measurable porosity. Martin has been able to design and synthesize several phosphonate linkers that oppose this trend. The linkers have been designed to be bulky and rigid, disallowing their ability to pack efficiently. Combined with the use of templating additives during their self-assembly, a diversity of porous solids have been synthesized. The connectivity of the overall network and the geometry of the pores are highly dependent on the identity of the added template. Upon template removal, the resulting MOFs are porous, and are highly selective to carbon dioxide over nitrogen, the major component in flue gas. This template-directed approach and the separating performance of the resulting MOFs will be reported in a future manuscript.

Final remarks

- The synthesis of these new porous solids was enabled by the discovery of new molecular building blocks, combined with the use of templating additives.
- Martin and his team are testing their new library of materials in more realistic flue gas chemical mixtures as well as other high-value chemical separations enabled by the receipt of an NSERC Research Tools and Instruments grant for competitive gas separation experiments.

Martin acknowledges CFREF, NSERC CREATE, NOVA chemicals, Alberta Graduate Excellence Scholarship, John D. Petrie QC Memorial Graduate Scholarship for funding and support.

Bioenergy

Alyse Hawley
Postdoctoral Fellow

Introduction

Dr. Alyse Hawley, PhD, works on understanding how metabolic interactions between microbes can help to better engineer microbial communities capable of efficient energy neutral carbon dioxide (CO_2) bioconversion. Engineered microbial communities include viruses that infect microbes, and further understanding of how viruses impact the microbe's metabolisms and interactions and the resulting outcome that has for CO_2 bioconversion. Further exploration of elemental cycling in Soda Lake, where microbes for bioreactors were sourced from, can also provide information to better understand how microbial interactions work to build strong engineered microbial communities for CO_2 bioconversion.

Results

Alyse has found that many viruses are present in the CO_2 bioconversion engineered community, but that they do not appear to significantly disrupt the stable functioning of the microbial community. Elemental cycling for carbon and nitrogen between microbes within the CO_2 bioconversion reactor appears to be central to sustaining the microbial community interactions and bioconversion process.

Final remarks

- Better understanding of microbial nitrogen cycling in alkaline conditions may address challenges for cost-effective CO_2 bioconversion under alkaline conditions.
- Viruses that infect microbes within stable engineered microbial communities may play critical roles in the stability of the community, leading to stable outcomes of engineered bioprocesses.

Bioenergy

The role of viruses in an engineered microbial process

Varada Khot
PhD student

Introduction

Under the supervision of Dr. Marc Strous, Varada Khot researches the ecology of viruses in an engineered algae community. Her research uses omics-based approaches to understand the relationship between the microbial community members and their viruses, and how the community has evolved resiliency to viral predation.

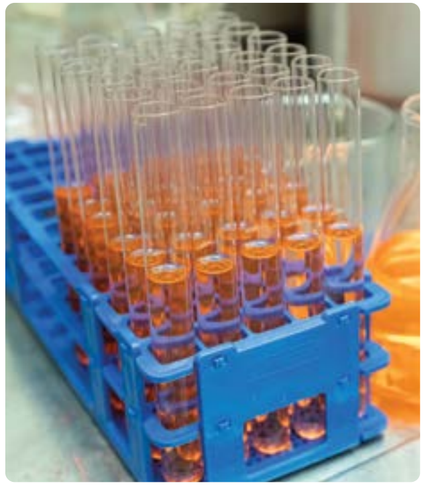
Results

From Varada's initial analysis of the microbial community grown in a photobioreactor in the lab, gene fragments representing approximately 50 individual viruses were identified from metagenomic data. As many as 15 viruses in this community are novel viruses with no known relatives. In addition, 16 microbial community members encode an adaptive defense system against viruses known as CRISPR-Cas, with the cyanobacterial population encoding at least five different systems. Varada's next project will be to look at the viruses from Soda Lake (from where this community originates) to understand how the viruses have evolved from the lakes to the photobioreactor in the lab.

Final remarks

- This population of cyanobacteria has many diverse CRISPR-Cas systems.
- Many novel viruses with no known relatives exist in the photobioreactor microbial community.

Stefan Lenz
Postdoctoral Fellow



Introduction

Organic photovoltaics (OPV) are attractive candidates that filter and convert light into electricity within clean energy photobioreactors. Despite OPVs having significant flexibility and colour tunability desirable for photobioreactors, OPV materials are often inefficient at converting non-transmitted light into electricity. The overarching goal of Dr. Stefan Lenz, PhD, and his team's research is to combine chemical intuition, cutting-edge experimental techniques and emerging artificial intelligence technologies to optimize and develop new efficient OPVs.

Results

Development of high efficiency OPVs is difficult to predict and dependent on several experimental conditions. Often only a small number of experimental conditions can be explored due to time and resource constraints, yielding sparse datasets. Therefore, methodologies that accurately suggest only promising experimental conditions to perform are highly valuable. To that end, Stefan's current role has been to use several machine learning techniques to suggest new, tunable production conditions that aim to maximize efficiency of a well-characterized OPV. Through this iterative and learning-guided process, optimum OPV production conditions are obtained and the theoretical maximum efficiency of an OPV material can be determined. The goal from this phase of the project is to use learning-guided experiments to maximize the efficiency of several OPVs. The next step in the project is to use machine learning to explore chemical space and predict high efficiency OPV materials that are yet to be synthesized.

Final remarks

- Machine learning techniques help visualize experimental data to identify underexplored regions of experimental space.
- The next step is to develop a machine learning platform to maximize the efficiency of OPV materials.

Bioenergy

William Richardson
Research Associate

Introduction

A 1000 litre outdoor algal pilot plant was constructed in 2019 to assess the economic viability of CO_2 conversion to bioenergy and bioproducts at a large scale. It was expanded to a 3500-litre pond reactor in the summer of 2020. Dr. William Richardson, PhD, provides operational and design support to the algal pilot plant team. His responsibilities include the operation and maintenance of the plant, design and prototyping of new unit operations and developing mathematical models of the plant.

Results

In the summer of 2019, the pilot plant was operated for 140 consecutive days. William showed that the bioenergy potential associated with the algal growth is higher than the energy requirement for compression in the system, validating it as an energy positive process. Using small-scale experimental data, he developed an algal growth model that accounts for light attenuation with depth in the reactor but not nutrient concentrations. During operation there was a sustained period of lower growth whose behaviour was not captured in this model. Analysis of the ion concentration showed that the period of low growth rate coincided with periods of high pH and the associated decreased iron solubility, iron being a limiting nutrient in this system. Maintaining a lower pH appears to be a critical operating parameter to achieve high growth rates.

Final remarks

- William has shown that the optimized algal growth process at the pilot scale is energy positive.

Bioenergy

Bioenergy production from microalgae

Taina Tervahauta
Postdoctoral Fellow

Introduction

The goal of this project is to convert solar energy into biofuel (methane) through microalgae cultivation and anaerobic digestion. Algae cultivation is done at high pH and alkalinity to improve carbon dioxide absorption and uptake. This however poses a challenge in the downstream processing of algae where high pH can induce ammonia inhibition during digestion. By using autofermentation as a pre-treatment step, the breaking down of algae biomass decreases the pH, minimizing ammonia inhibition during digestion. Additionally, this process can increase revenue by recovering value-added products from autofermentation. One of the main challenges is to implement successful recycling of carbon dioxide and nutrients to make biofuel production from algae economically feasible.

Figure 1

Results

Anaerobic digestion of microalgae can be performed most energy-efficiently at ambient temperatures, thus avoiding the energy consumption for heating the digestor. Digested manure and sewage sludge are commonly used inoculums for anaerobic digestion but are unable to perform at lower temperatures (below 35 C). Soda Lake sediment is the most suited inoculum for digestion of microalgae at an ambient temperature (21 C).

Continuous digestion of autofermented algae with Soda Lake sediment has been successfully operated for 213 days at an ambient temperature of 21 C, shown in Figure 1. The maximum methane yield achieved is 305 millilitres of methane per mass of algae, but the yield fluctuates with the ammonia concentration in the digestor.

Final remarks

- Increased concentrations of ammonia inhibit microorganisms in Soda Lake sediment, decreasing methane production from microalgae.
- Repeated inoculation rounds with Soda Lake sediment show increased methane production suggesting adaptation of the microorganisms to higher ammonia concentrations.

Bioenergy

High voltage organic photovoltaics for greenhouse applications

Francesco Tintori
PhD student

Introduction

The main goal of Francesco Tintori's project is developing a printable organic photovoltaic (OPV) system that can be scaled up to large areas and industrial quantities. This system is to be red in order to absorb blue radiation that is damaging to the algae in the bioreactor. The organic photovoltaic devices also need to have good efficiency in producing electricity, and in this regard, a high-voltage system is being targeted to increase the power output of the photovoltaic cells.

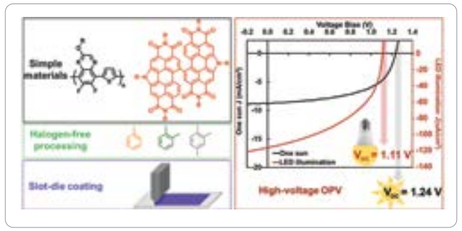


Figure 1

Results

A red-coloured semiconducting polymer (PTQ10), which has a scalable high-yielding synthesis and is commercially available, was selected to be used in a system with the red-coloured perylene diimide (tPDI$_2$N-EH) material. The chemical structures can be observed in Figure 1 as well as their blended absorption profile, Figure 2, which shows the absorption of blue light. The organic photovoltaic devices fabricated using the scalable technique of slot-die coating were tested under simulated sunlight to give a power conversion efficiency of around six per cent, but most importantly, a very high open circuit voltage of 1.2 volts. These results are significant because the photoactive materials were processed and tested in air, using large-scale compatible solvents and techniques. The high voltage also allowed for a secondary application of the photovoltaic cells, which is indoor light recycling. Cells under low-intensity LED bulbs could still produce voltages as high as 1.1 volts, which is a remarkable achievement.

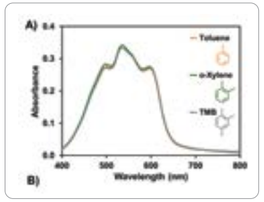


Figure 2

Final remarks

- The studied system has potential for industrial-scale production, which is required for applications such as the implementation in a bioreactor. This is both from the materials and the fabrication point of view.
- The system is red-coloured, which can act as an efficient filter for the blue light that is harmful for algae and produce electricity at the same time.
- The high voltage obtained with this system makes it a candidate for other applications.

Bioenergy

Optimisation of non-fullerene acceptors (NFAs) in organic photovoltaics (OPVs) via machine learning

David Turnbull
MSc student

Introduction

The overall goal of David Turnbull's team is to create a clean energy photobioreactor capable of reducing CO_2 emissions and generating high value-added products. Organic photovoltaics (OPV) have been identified as a perfect matching technology because of their lightness and flexibility, making them adaptable to the various form factors present in the photobioreactor, and their colour-tuneability, enabling selective transmission of the appropriate photons that promote algae growth and conversion of the non-transmitted light into electricity. The project thus involves the development of large-area red transparent OPV, acting both as light filters and collectors/convertors, leading to a self-powered photobioreactor.

Results

David's role in this project is to develop an approach to rapidly produce novel photovoltaic acceptors for use with machine learning to optimize the photovoltaic cell performance. Several approaches have been explored so far, with two ruled out for being unsuitable for various reasons. David has also been using data from collaborators at the University of Victoria, and they have confirmed that a particular machine learning approach looks promising for predicting self-assembly from limited amounts of experimental data. The next steps of David's research are to synthesize new molecules in a combinatorial fashion and to test performance.

Final remarks

- David has found the appropriate molecule design for use with machine learning.
- The materials are typically high performing and might be useful as a tertiary component in photovoltaic cells.
- David confirmed that a particular machine learning approach looks promising for predicting self-assembly from limited amounts of data.

Bioenergy

Economical and sustainable process for production of phycocyanin — a high value natural product

Agasteswar Vadlamani
Postdoctoral Fellow

Introduction

Though bioenergy with carbon capture and storage (BECCS) is recognized as a potential negative emission technology, large-scale implementation of BECCS with current technologies would compromise food production. Bioenergy and bioproducts derived from phototrophic microorganisms, with direct capture of CO_2 from air, could overcome this challenge.

Dr. Agasteswar Vadlamani, PhD, aims to achieve higher biomass productivities while simultaneously capturing atmospheric CO_2. His goal is to develop a bioprocess that would lead to extraction of high-value products in a more economical and sustainable way.

Results

Agasteswar has demonstrated that the cyanobacterial consortium obtained from the alkaline Soda Lake was able to grow at high pH (up to 11.2) and alkalinity (approximately 500 millimoles per litre). The biomass productivity was higher or comparable to previously reported values for alkaliphilic microalgal cultures. Further, the pH swing during the algal growth (10.5-11.2) enabled effective regeneration of the growth medium by direct CO_2 capture from air.

Agasteswar has filed a patent about the bioprocess to simultaneously extract and purify phycocyanin — a natural blue colour — from wet algal biomass.

Final remarks

- In 2019, Agasteswar completed a provisional patent application.
- This innovation led Agasteswar to co-found Synergia Biotech Inc., a cleantech start-up focused on developing an innovative approach to cultivate, harvest and extract phycocyanin.
- The Synergia Biotech team has successfully graduated from the Prime stream at Creative Destruction Lab-Rockies (CDL).

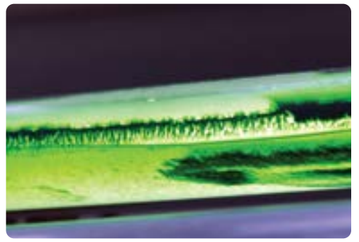
Bioenergy

Sustainability analysis of biological carbon fixation (algae technology) through computational tools

Ahasa Yousuf
PhD student

Introduction

Microalgae are unicellular organisms that exhibit high photosynthetic efficiency and are thus helpful for CO_2 fixation. Furthermore, algal biomass can be utilized to produce biofuels and value-added chemicals. Ahasa Yousuf's project aims to develop a model that will address the economic and environmental sustainability of the pathways and challenges associated with the large-scale implementation of the microalgal cultivation and conversion system. The aim is to use computational tools to develop growth, kinetic and conversion models to be able to replicate experimental and pilot-scale results. The model will lead to optimized cultivation conditions and will help to design a sustainable pathway for converting CO_2 and algae into valuable products.



Results

To achieve the project goal, a mathematical model of a flat panel reactor was developed. The model predicts temperature and light profile as a function of reactor height, length, width and biomass concentration, and its effect on algal productivity. Temperature has been identified as a critical factor and a range of 20-35 C appears to be necessary for algae to thrive; deviation from this temperature range could significantly decrease algal productivity. Algal productivity is low from November to February because of extreme cold conditions in Alberta. Algal productivity is linearly correlated with length, height, width and biomass concentration. However, for width, there is a threshold point after which productivity decreases due to photoinhibition. Finally, reactor configuration is likely to critically influence algal productivity. Thus, Ahasa aims to develop models of different reactor configurations, and to evaluate the optimum geometry that maximizes productivity.

Final remarks

- The model incorporated the influence of solar irradiance, temperature, and nutrients as a function of reactor geometry, and needs to be verified with outdoor photobioreactor for its effectiveness.
- Temperature control and reactor geometry play a crucial role in the development of a sustainable algae cultivation system.
- The model could be a useful tool in designing an optimum biomass production system.
- Future work targets the modelling of different reactor configurations, conversion of algal biomass to valuable products and a sustainability evaluation of the technology.

Bioenergy

An integrated approach to improving efficiency in microbial biofuel systems

Jackie Zorz
PhD student

Introduction

Jackie Zorz's research focuses on improving and understanding the algae-for-biofuel system. One of her goals is to determine the feasibility of integrating organic solar cells, for electricity generation, with the growth of algae. Another research aim is to investigate a patented process that results in algae lysis and the release of a large quantity of a highly-valued product, phycocyanin. She is interested in what is happening at the molecular level during this process.

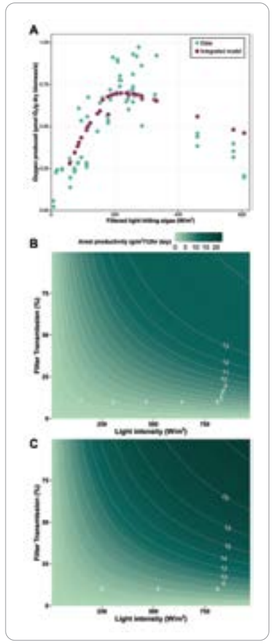
Results

The use of an organic semiconducting material to partially filter the light reaching an algae bioreactor was an exciting proposition because it meant that excess light energy could be captured by an organic semiconducting material and converted to electricity. This also shields the algae bioreactor from potentially damaging levels of light, allowing for better growth. Through experiments and modelling, Jackie and her team found that algae growth is more often negatively affected by light limitation and light attenuation in a bioreactor than by light inhibition due to too much light. Thus, a combination of organic solar cells and an algae bioreactor system will only be beneficial to algae growth if the algae density is low, the light intensity is very high, or if the bioreactor is shallow.

Through investigation of molecular components like proteins and DNA, Jackie is trying to explain what causes the algae cells to break apart and release phycocyanin, a valuable blue pigment, after incubation in the dark. She has been able to confirm that the lysis is not due to predation or a viral attack but appears to be an automatic mechanism of the algae.

Final remarks

- Through work on algae growth and light filtration, Jackie has concluded that filtering incident light with a red organic semiconducting material is only beneficial for algae growth under conditions with high light intensity or low algal density.
- For other conditions, either a thinner bioreactor, or an organic semiconducting material with absorption properties outside of the visible spectrum of light (i.e., infrared) are recommended.
- The algae lysis in the phycocyanin releasing process appears to be caused by an internal mechanism rather than through predation from other bacteria or a viral attack. This research is ongoing.



NEGATIVE EMISSIONS PETROLEUM SYSTEMS (DIRECT AIR CAPTURE/ EOR, ETC.)

Sean McCoy, Steven Bryant, Nader Mahinpey, George Shimizu, Hector De la Hoz Siegler, Joule Bergerson, Anne Benneker, Samira Siahrostami, Michelle Dolgos, Md. Golam Kibria

Background

Scientific consensus holds that effective strategies for mitigating climate change must include technologies for negative emissions of carbon dioxide (CO_2) in addition to technologies for avoiding GHG emissions. Currently there are very few options for scalable, rapidly deployable net negative emissions technologies (NETs). This project has described a novel NET which combines direct air capture (DAC) with storage of CO_2 and production of brine and energy from a subsurface reservoir. Crude oil is the energy form most likely to be feasible. This proposal addresses research questions arising from this combination of technologies.

Research strategy

This strategy is defined by two phases. In the first phase, an HQP "tiger team" is working to identify elements of the combined DAC-CO_2 storage and oil production technology where technical improvements would have greatest impact on scalability, deployment and carbon negativity of the combined technology. In parallel, five HQPs have been recruited to attack different areas that are anticipated to result in significant improvements. In the second phase of the project, the tiger team analysis will be used to define additional projects (and recruit additional HQP) that will accelerate development and deployment of the DAC-CO_2 storage system. This two-phase approach has been chosen as it is not obvious a priori which innovations will have the greatest potential to advance the concept. This research program is being conducted in parallel with efforts to organize a field demonstration of this NET.

Desired outcomes

This research project is anticipated to lead to innovative technical solutions, such as novel adsorbent materials, structured packings, manufacturing and operational strategies — that reduce the cost of negative emissions and make it more easily scalable. Its is also expected that these results will strongly inform the design of a potential technology demonstration and will set a course for further research. It is also intended to engage companies in the oil and gas sector to consider how they can advance development and deployment of negative emissions technologies.

Negative emissions petroleum systems (Direct Air Capture/EOR, etc.)

Akram Alabsi
PhD student

Introduction

Akram Alabsi's project aims to synthesize, characterize and evaluate new efficient, scalable and cost-effective adsorbents which effectively capture CO_2 from the atmosphere for use in enhanced oil recovery (EOR).

Results

Currently, Akram is in the process of reviewing literature to figure out the current developments in supports, functional groups and types of reactors being used to evaluate the capacity and selectivity of the adsorbents. He is also preparing the best design of the experimental setup.

Final remarks

- Due to the early stage of his project, Akram still does not have clear conclusions from the literature review.

Negative emissions petroleum systems (Direct Air Capture/EOR, etc)

Assessing the potential scale and benefits of direct air capture (DAC) and CO_2-EOR as a negative carbon emission technology

Shima Bashti Monfared
PhD student

Introduction

In her research, Shima Bashti Monfared will investigate a novel negative emission technology (NET) that integrates direct air capture (DAC) with underground storage of CO_2 through enhanced oil recovery (EOR), enhanced gas recovery (EGR) and enhanced geothermal energy recovery (EGER). She intends to achieve lower carbon emissions and higher oil recoveries.

Results

Shima is developing an integrated system for the analysis of coupled DAC and EOR processes from an exergy-balance perspective. She is evaluating whether and under which conditions it is exegetically effective to store CO_2 through EOR. This model is also used to identify opportunities to increase the efficiency of the combined process through better integration of DAC and EOR. The preliminary results show that the exergy analysis of integrated direct air capture (DAC) and EOR identifies the equipment/processes with low efficiency. Process performance can be improved by potential efficiency optimization of resources and equipment usage uncovered through exergy analysis. This project presents insights in moving toward an economically-robust and environmentally-sustainable CO_2-EOR process.

Final remarks

- Shima is working on identifying the DAC technology suited for integration with EOR, EGR (and possibly EGER).
- She is developing coupled surface-subsurface management strategies for sustainable negative emission DAC-EOR processes with potential near-term economic viability.
- Subsystems in the coupled systems that, through their improvement, would have the largest impacts on the economics and life cycle of the overall system will be identified.
- This model and findings from the earlier phase of the work will be used to estimate the negative emissions potential for EOR and EGR in Alberta, and possibly globally.

Negative emissions petroleum systems (Direct Air Capture/EOR, etc)

Promoting H_2O_2 production via 2-electron oxygen reduction by coordinating partially oxidized Pd with defect carbon

Amir Hassan Bagherzadeh Mostaghimi
MSc student

Introduction

Electrochemical synthesis of H_2O_2 via a two-electron oxygen reduction reaction is proposed as a promising method for on-site water purification. The objective of this project is to develop electrocatalysts that can efficiently produce H_2O_2. This project shows that small palladium (Pd) clusters loaded in partially-oxidized carbon nanotubes fulfill this purpose. This work is a collaborative experimental and computational project between the University of California San Diego (UCSD) and the University of Calgary/CFREF. Amir Hassan Bagherzadeh Mostaghimi modelled the reaction on several simulation models to unravel the active site and shed light on the mechanism of the reaction at the atomic level using density functional theory calculations.

Results

Experimental results at UCSD show that loaded palladium clusters in partially-oxidized carbon nanotubes are highly active and selective for synthesizing H_2O_2.

Amir simulated models of several defective graphene sheets with embedded palladium clusters in different sizes using an atomic simulation environment code. Then, he simulated the oxygen reduction reaction on the built models using a Quantum Espresso simulation package to understand the surface structure during the reaction and the possible active sites involved. The results can be summarized in an activity volcano map in which the highest activity is achieved on the pick of the volcano. This analysis shows Pd_3 and Pd_4 clusters surrounded by oxygen functional groups show the highest activity. This indicates a synergy effect between Pd_3 and Pd_4 clusters and oxygen functional group. The results of this work have been recently published in *Nature Communications*.

Final remarks

- The product selectivity of amorphous palladium loaded into partially-oxidized carbon nanotubes was observed to be nearly 100 per cent.
- The outstanding performance of the electrocatalyst was maintained during an eight-hour period of test time.
- The Pourbaix diagram analysis of the structure revealed that the surface of the electrocatalyst is covered with oxygen groups. These groups are found to make the bonding energy more favourable towards H_2O_2 electrosynthesis.
- Functional groups on the carbon sheet (epoxy-functional groups) are maximizing the selectivity of the surface. These results revealed a synergetic interaction between the oxygen functionalized carbon and the palladium cluster.

Negative emissions petroleum systems (Direct Air Capture/EOR, etc)

Investigating optimum cost strategies to decarbonize hydrogen production in Alberta

Abdalla Elnigoumi
MSc student

Introduction

The goal of the project is to identify the best (economic/environmental) options to decarbonize hydrogen (H_2) production in Alberta. Abdalla Elnigoumi aims to do so by conducting economic assessments on different H_2-production options, such as steam methane reforming (SMR) and autothermal reforming (ATR), with varying CO_2 capture rates (60-90 per cent). He aims to evaluate the impact of several factors including scale and location of both H_2 production and CO_2 storage options in Alberta.

Results

Abdalla has developed an economic tool using Excel that estimates the levelized cost of H_2 and the amount of CO_2 emissions avoided for three plant configurations (SMR with pre/post carbon capture and ATR with pre-carbon capture). This economic tool will be used in conjunction with others to study plausible hydrogen supply and demand scenarios, and to identify trade-offs at system and component levels to build the best fit decarbonization strategy.

Final remarks

- The decision of whether to prioritize environmental or economic benefits will influence the choice of the decarbonized H_2 production configuration.
- The capacity and location of CO_2 storage options will have a pronounced effect on the pipeline cost and therefore the overall model, which raises the need to address uncertainties in this aspect.
- The SMR model with 60 per cent capture has the lowest prediction using the high resolution deterministic prediction system (HRDPS), followed by the ATR and lastly, the SMR with 90 per cent capture rate.

Negative emissions petroleum systems (Direct Air Capture/EOR, etc)

Absorbent materials design

Evan Gabert
PhD student

Introduction

Evan Gabert's work focuses on the design of new adsorbent materials to capture CO_2 from the atmosphere. The captured CO_2 can then be stored, used for enhanced oil recovery, or converted to useful chemicals. These adsorbent materials could be used as part of a carbon-negative process to counteract CO_2 emissions. This project involves the synthesis of novel metal-organic frameworks (MOFs) with enhanced selectivity for CO_2 over other atmospheric gases. Some key challenges of this work include efficient extraction of CO_2 from low atmospheric concentrations and ensuring adsorbent stability over many cycles.

Results

Evan has continued to develop novel methods for the creation of stable CO_2-selective MOFs. Specifically, he is studying a system that can change structure in response to the presence of different molecular templates. The resulting MOFs have demonstrated excellent thermal, acid and water stability. While different structures can be formed with different templates, an important question is whether the molecular pores are actually imprinted with the shape of the template. Experiments assessing the ability of the template to enhance selectivity are underway.

He is also studying the use of CO_2 as a template to induce selectivity. He synthesized several linker molecules which will result in more favourable CO_2 templating. He is interested in forming MOFs from these molecules and looking forward to measuring their CO_2 selectivity.

Final remarks

- Evan demonstrated the flexibility of the novel MOF synthesis method to accept several different templates. This method could result in a new widely applicable technique to promote gas adsorption selectivity and apply this to direct air capture of CO_2.
- The template used in this method can greatly impact MOF properties such as stability and gas adsorption.
- Several stable MOFs have been produced for ongoing CO_2 selectivity measurements.

Negative emissions petroleum systems (Direct Air Capture/EOR, etc)

Techno-economic assessment of carbon capture and utilization technologies in the Canadian context

Benjamin Lincoln
MSc student

Introduction

Benjamin Lincoln's goal is to assess the feasibility of carbon capture and utilization (CCU) projects in the Canadian industrial landscape using techno-economic assessment methods. These projects could have the potential to offset the financial burden of climate change mitigation technologies through the creation of a value-added product directly from the captured carbon dioxide. Benjamin is aiming to study a variety of models in literature and adapt them to a Canadian context to better understand the applicability of these projects to our economic future.

Results

Benjamin has begun the creation of an Excel-based assessment tool with the intent of normalizing the financial assessment of literature models. It has become evident that the variety of financial assessment methods in literature is an issue. It is important to understand the potential of each CCU project on identical financial bases to streamline decision making for the allocation of research resources. By creating a standardized cash flow analysis tool, the comparison of these technologies should be simplified greatly. Further research will be applied to the preliminary assessment of CCU pathways that have relatively lower technology readiness levels, or for the creation and sale of products that have not been assessed in literature. Results will be in the form of comparative reports between CCU pathways and an assessment of the potential that each of these pathways has within Canadian markets.

Final remarks

- Benjamin will create a cash flow analysis tool for the assessment of literature on CCU models with the ability to tailor the financial context to a variety of locations within Canada.
- Benjamin will assess the feasibility of low technology readiness level pathways for CCU using engineering first principles.
- This research hopes to inform Canadian researchers and create a framework in which techno-economic results can be easily compared.

Negative emissions petroleum systems (Direct Air Capture/EOR, etc)

Comparative life cycle assessment of electrochemical upgrading of CO_2 to fuels and feedstocks

Shariful Kibria Nabil
MSc student

Introduction

Shariful Kibria Nabil's project aims to compare cradle-to-gate life cycle assessment (LCA) of one-step (CO_2-to-products) and two-step (CO_2-to-CO-to-products) electrochemical conversion of CO_2 for eight major value-added products, considering CO_2 capture, CO_2 conversion and product separation in the comparative model. Shariful Kibria intends to measure the carbon intensity (i.e., global warming impact) of the electrochemical routes in comparison to the thermochemical CO_2 utilization route and the fossil fuel-based conventional synthesis route for those same products. He hopes that this analysis will guide the CO_2 electro-reduction community to target technological goals achievements, such that when coupled with low carbon electricity, the electrochemical routes would bring climate benefits in the near future.

Results

This study found that the energy required for CO_2 capture contributes only one to eight per cent of the overall energy requirement and associated CO_2 emissions for the electrochemical CO_2 utilization route. Higher global warming impact for the electrochemical process, due to intensive energy requirements for electrochemical conversion (60-80 per cent of total energy) and product separation (70-80 per cent of total energy), were found for gas and liquid products, shown in Figure 1 and Figure 2. However, electrochemical processes can potentially incorporate intermittent renewable energy and, following the projection by the Energy Information Administration (EIA), Shariful identified that the minimum percentage of renewable energy share in grid electricity (approximately 40 per cent) needed to get the near-term environmentally-compelling products from electrochemical route will be achieved by 2040, shown in Figure 3.

Final remarks

- Shariful's main goal is to perform a comparative life cycle assessment between electrochemical, thermochemical and conventional processes.
- The electrochemical process is dependent on electrical grid intensity.
- Shariful has identified environmentally sustainable electrochemical products (near-term and long-term).
- The project will reveal the technological goals and challenges faced by the electrochemical process to compete with thermochemical and conventional processes.

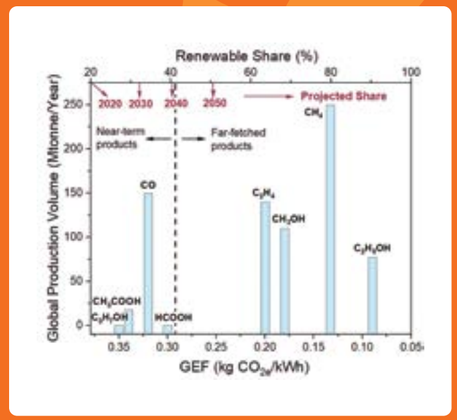


Figure 1

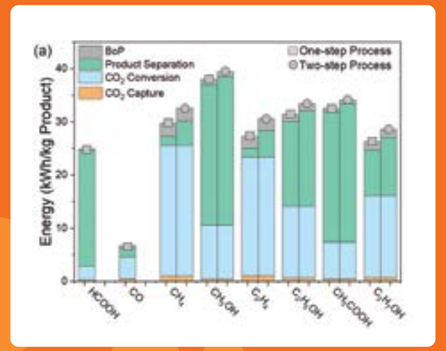


Figure 2

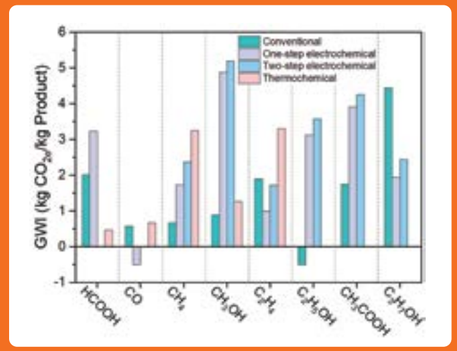


Figure 3

Negative emissions petroleum systems (Direct Air Capture/EOR, etc)

Evaluating direct air capture and sustainable energy generation for climate change mitigation with life cycle and techno-economic assessment methods

Ayesha Shaik Khaja Mohiddin
PhD student

Introduction

Ayesha Shaik Khaja Mohiddin aims to provide a technically grounded recommendation framework for policy makers and investors in the climate change and energy policy arenas. The end goal is to remove the barriers against the deployment of carbon dioxide removal methods from the environment using sustainable energy. She is building a performance model for direct air capture (DAC) systems combined with energy generation, with process- and systems-level optimization. Higher level analyses included in this project are sensitivity analysis, life cycle and techno-economic assessments.

Results

Ayesha is applying a combined analytical and numerical approach towards ambient air decarbonization projects by using analytical modelling methods in conjunction with process engineering fundamentals, supplemented with Aspen modelling and spreadsheet-based models. Modelling the air contactor and regeneration of the capture media (primarily solvent- and sorbent-based DAC) is the first phase. The foundation of the model is a direct air capture and storage system integrated with multiple energy generation options (e.g., enhanced oil recovery (EOR) and co-generation of geothermal energy from the produced water, natural gas, electric grid supply, other renewables, etc.).

Final remarks

- Ayesha has analytically modelled an air contactor for a solvent-based direct air capture system at a slab level, comparable to carbon flux equations provided for current commercially operated direct air capture air contactors. The next step for a solvent-based system is configuring the regeneration loop.
- Comparisons of the carbon capture loops for solvent and sorbent direct air capture systems show a significant disparity in the energy requirements. Further analysis is required to understand the trade-offs in process inefficiencies.
- Sensitivity analyses of sorbent-based direct air capture systems show that sorbent material, energy and carbon intensity are among the most impactful parameters affecting the net negativity of direct air capture and storage systems.

LOW CARBON TECHNOLOGY ASSESSMENT/INVENTION/ INNOVATION USING BIG DATA

This project is conducted by the University of Calgary Technology Assessment and Coordination Team (TACT)

Steve Larter, Ian Gates, Alexander Whalley, Innovate Calgary

Background

The importance of low carbon technology for the environmental and economic future of the planet is clear. Yet there is little cross migration of concepts and elements from widely disparate fields into the petroleum sector and little game changing, or breakthrough innovation is occurring. This project aims to answer whether big data solutions to technology analysis and invention are possible?

Research strategy

This project will develop tools based on recently available big data on patents. The analysis tools will have two objectives. The first objective will be the development of a technology markup language (TML), and definition algorithm for a fundamental technology element (FTE). The second objective will be the creation of an impact analysis of energy technologies tool. These tools will allow innovation managers in both private and public sectors to find new low carbon technologies that have significant market potential. This research seeks to speed up commercialization of effective low carbon technologies. The project will initiate a new interdisciplinary collaboration between faculty in Petroleum Engineering, Geoscience and Economics. The combination of deep understanding of technologies – oil recovery and decarbonisation– with automated patent analysis and economic valuation of patents presents a unique intellectual opportunity to disrupt business as usual in the academy and in society.

Desired outcomes

The tools proposed will enable assessment of the market potential at early stage thus providing dramatic increase of returns to research activity in low carbon technologies. This tool would be invaluable for both private and government stakeholders; and has the potential to revolutionize how research activities are funded. A low carbon technology markup tool could also guide policy makers in tracing important technologies back to basic R&D investments and learning what institutional structures can maximize the commercialization of promising ideas.

Algorithms and software for patent and technology analysis (TML, FTE) are some of the expected technical outcomes, as well as a report on the feasibility of using big data to measure the market potential of early stage low carbon technology ideas. It is likely that commercially valuable IP will be generated in this project and it will be appropriately protected in collaboration with Innovate Calgary. Software development and prototyping of tools that could be licensed to government, high tech companies, or law firms are also anticipated.

Low carbon technology assessment/ invention/innovation using big data

Real time low carbon technology assessment using patent sentiment analytics

Amir Hallak
MSc student

Introduction

Amir Hallak's project is to create a software tool that uses economic theory and machine learning algorithms to identify valuable carbon-reducing patents in real time.

Results

Dynamic codes have been created that would grab the newest set of granted patents and update the current working database. These datasets are cleaned and prepared using python codes and then fed into machine learning regression equations and text analysis algorithms. Therefore, the patents are evaluated in real time and the results are promising when compared to actual patent evaluating companies.

Final remarks

- Different kinds of datasets have been created from acquired raw data.
- Datasets have been cleaned and disambiguated as to be more productive and useable than the existing datasets.
- Since there is no market for patents, it is important to create a system that evaluates patents for small businesses and inventors rather than having them pay thousands of dollars to law firms.
- The final goal of this project is to create a software tool that would help small businesses and inventors have an idea on how much their patents are worth with a focus on carbon-related fields.
- The final software will present the user with an estimate on the patent, related patents and other important information.

Low carbon technology assessment/ invention/innovation using big data

Real time low carbon technology assessment using patent sentiment analytics

Gilbert Lybbert
MSc student

Introduction

Gilbert Lybbert's project is to create a patent information and valuation tool to identify emerging low carbon technologies with high potential in real time.

Results

He has developed a process to dynamically collect, clean and prepare a large quantity of patent data from various sources. This data is then used in a machine learning model to predict the value of each patent.

Final remarks

- He has compiled a valuable set of data which has been cleaned and disambiguated to be more comprehensive and directly useable than existing datasets.
- He has identified the major factors that contribute to the value of a patent.
- Using this data, the final software tool will allow a user to find a patent by company or classification, and retrieve information about its value, key features and related patents.

Low carbon technology assessment/ invention/innovation using big data

Mohsen Ramezanpour
Postdoctoral Fellow

Introduction

Dr. Mohsen Ramezanpour, PhD, aims to develop algorithms for finding high-impact and disruptive low carbon technologies. Using these algorithms, game-changing low carbon technologies will be identified, valuated and classified according to their impact on reducing the greenhouse gas emissions. Mohsen also aims to develop algorithms for acceleration and automation of low carbon technology innovation to identify, transfer and use the innovative elements from other domains in the invention of noble low carbon technologies and solutions to assist in reducing greenhouse gas emissions.

Finding the disruptive and game-changing low carbon technologies with real impact is challenging. Despite many technologies available, and many more appearing every day, only a small percentage are actually clean technologies and could be disruptive.

Most clean technologies have been developed by companies outside the energy sector. This strongly suggests and supports the idea that the innovation elements for clean energy technologies are already available in other domains. However, to use those elements in the energy sector to accelerate the innovation of new low carbon technologies, the elements need to be identified.

Results

Mohsen has already developed a version of the predictive model. This version of the algorithm can be used to identify the leading companies in green technology and their disruptive low carbon technologies, valuating those technologies and ranking them based on their impact. This algorithm has an acceptable level of precision for the desired application, although further improvement (version 2.0) is currently under development. The second version is expected to have a significant improvement over version 1.0 in terms of prediction accuracy.

Mohsen has also worked on and developed the initial version of the algorithm to identify the innovative low carbon-related elements from other domains, which could assist in developing new low carbon technologies. This algorithm is still under development.

Final remarks

- The first version of the algorithm shows a great promise in finding low carbon technologies, valuating them, and ranking them based on their impact and disruptiveness.
- Given the large number of technologies available, an automated machine-based approach is a promising approach in extracting and transferring such innovative elements to the green technology and eventually reducing greenhouse gas emissions.

UNIVERSITY OF CALGARY & UNIVERSITY OF ALBERTA JOINT PROJECTS

Both the University of Calgary and the University of Alberta share a common drive to build a low carbon and energy-efficient Canada, thus creating an example in the global scenario. Both universities are combining their strengths and world-leading researchers to propel Canada towards a sustainable future. In 2016, the Canada First Research Excellence Fund (CFREF) invested a total of $150 million into the province, with $75 million allocated to the University of Calgary and $75 million allocated to the University of Alberta. As part of the awards, a portion of the two funds, $6.5 million each, were allocated from the two universities to create collaborative research projects that are within the mandates of the two CFREF research programs. To date, the two universities have created nine collaborative projects, involving more than 20 faculty members, with more than 30 graduate students and postdoctoral scholars. The universities have held five large joint workshops (winter 2017, winter 2018, fall 2018, winter 2019, fall 2019) for updating research progress collectively to the joint project participants.

University of Calgary faculty members involved in the projects in this section are Profs. Joule Bergerson, Viola Birss, Steven Bryant, David Eaton, Ian Gates, Hersh Gilbert, Hassan Hassanzadeh, Hossein Hejazi, Josephine Hill, Jinguang Hu, Kristopher Innanen, Apostolos Kantzas, Donald Lawton, Bernhard Mayer, Giovannianotonio Natale, Sathish Ponnurangam, Venkataraman Thangadurai, Melanee Thomas, Simon Trudel and Harvey Yarranton.

ADVANCED ELECTROCHEMICAL SYSTEM FOR ENERGY STORAGE THROUGH CO_2 CONVERSION

UCalgary Team: **Viola Birss**, Joule Bergerson, Sathish Ponnurangam, Simon Trudel, Venkataraman Thangadurai

UAlberta Team: **Jingli Luo,** Zhehui Jin, Qingxia Liu

Background

Solid oxide electrolysis cells (SOECs) can run on (and thus store) grid or distributed electricity produced from conventional hydrocarbons or from renewable electricity made by converting CO_2 to fuels that can be used to generate energy on demand and would be secure for long periods of time. University of Calgary and University of Alberta teams have independently developed some very promising catalytic mixed conducting electrode materials for use in SOECs. The group has succeeded in optimizing the SOECs' operating temperature to 800 C. However, there is much more work needed in terms of further improving the performance of the catalysts, better understanding the reaction mechanism, lowering the SOEC operating temperature to simplify the engineering requirements and also varying the CO_2 gas composition to tune the product distribution.

Research strategy

Lowering the operating temperature of the SOECs will simplify cell operation and lengthen the lifetime of the SOEC components. The effect of tuning the composition of the syngas produced by the electrolysis of CO_2 and steam and how the input gas composition (CO_2:steam ratio) influences catalyst activity and stability as a function of operating temperature and cell voltage will be examined. Density functional theory (DFT) simulations using the Vienna Ab-initio Simulation Package, as well as Reactive Molecular Dynamics calculations, will be carried out to study the interactions of perovskite catalysts with CO_2 to help determine the mechanism of CO_2 adsorption and activation on the catalyst surface, and to calculate the energies of CO_2 adsorption and dissociation. As well, advanced surface science methods will be used at the Synchrotron facility in Saskatoon to determine the state of the catalyst surfaces during cell operation. Finally, an attempt to scale-up the SOEC cells will be made. A life cycle assessment (LCA) will also be undertaken to identify the unintended consequences of any new materials that are developed and issues related to cell scale-up.

Desired outcomes

The primary outcome of this research will be a stable, high performing solid oxide electrolysis device that demonstrates tunable syngas production from CO_2 and steam at the cathode and emits a pure O_2 stream at the anode, while also serving to store renewable and excess grid electricity. A second major goal of this research is to enable the scale-up of the cells by a factor of roughly 25 times in area, with guidance also obtained by detailed life cycle assessment. Cell optimization, advanced theory and surface science experiments will allow leading edge insights to be obtained, thus helping with knowledgeable modification of catalyst composition and other fundamental factors.

Advanced electrochemical system for energy storage through CO_2 conversion

Haris Ansari
Postdoctoral Fellow

Introduction

This project involves CO_2 conversion to useful chemicals using high temperature solid oxide electrolysis cells (SOECs). While the $La_{0.3}Ca_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$ (LCFCr) catalyst developed by the Birss group is already very active for CO_2 reduction/CO oxidation and oxygen reduction/evolution reactions, Dr. Haris Ansari, PhD, aims to enhance the electrochemical performance of LCFCr by doping it with nickel (Ni), followed by reduction in H_2 to form exsolved Fe-Ni alloy nanoparticles anchored to the LCFCr surface. His work involves stability studies of the nanoparticle modified catalysts in CO_2/CO environments and their impact on the activities for both CO_2 reduction and CO oxidation.

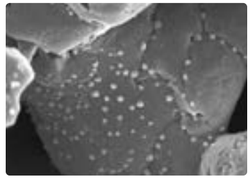


Figure 1

Results

Haris has shown that Fe-Ni nanoparticle-decorated LCFCr are resistant to coke formation and stable in CO_2/CO environments without appreciable changes in their size or composition in environments containing a high CO content. Symmetrical cells were prepared by depositing approximately 20-micrometre thick electrode layers of Ni-doped LCFCr on both sides of the cell. The cells were heated to 800 C and the fuel electrodes were reduced in 5 per cent hydrogen-95 per cent nitrogen (5%H_2-95%N_2) for two hours prior to cell operation. Scanning electron microscope (SEM) analysis revealed that the nanoparticles are approximately 50 nanometres in size and uniformly distributed on the catalyst surface, shown in Figure 1. The cyclic voltammetry (CV), depicted in Figure 2, revealed that the Fe-Ni nanoparticle modified catalysts exhibit a significant enhancement in activity for both CO_2 reduction and CO oxidation by approximately 30 per cent and 75 per cent, respectively, compared to the parent material. The high activities for both CO_2 reduction and CO oxidation make the material suitable for application in reversible solid oxide cells.

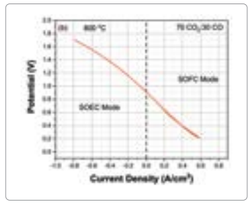


Figure 2

Final remarks

- Uniformly distributed and sized similar, (approximately 50 nanometres) Fe-Ni alloy nanoparticles can be exsolved from Ni-doped $La_{0.3}Ca_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$ (LCFCr) by reduction in 5%H_2-95%N_2 at 800 C.
- The nanoparticles are anchored to the LCFCr surface that enhances their stability in CO_2/CO containing environments and resistance to coke formation.
- One paper has recently been submitted regarding the stability of the parent compound in CO_2/CO environments and a second paper is in the pipeline on the topic of the effect of the Fe-Ni nanoparticles on both CO_2 reduction and CO oxidation.

Advanced electrochemical system for energy storage through CO_2 conversion

Conversion of CO_2 to syngas using perovskite-based solid oxide electrolysis cells

Irfan Aydogdu
PhD student

Introduction

Irfan Aydogdu aims to understand the degradation mechanisms of a perovskite-based electrocatalyst in solid oxide electrolysis cells (SOEC) to convert CO_2 and H_2O to syngas (CO and H_2). This project's focus is to develop a realistic model of a perovskite-based material via quantum mechanical tools. This model enables the exploration of how the electronic structure and redox stability of the electrocatalyst, impurities in reactant gases, and operating temperatures affect the stability of the electrocatalyst. The model also provides an opportunity to understand the variables that control the electrochemical CO_2 reduction mechanism.

Results

The result obtained so far is a developed reactive force field based on density functional theory (DFT) for strontium (Sr). The reactive force field is cross-validated by capturing the crystal phase transition of Sr under standard pressure and phase transition temperature conditions. The Sr reactive force field is used to develop reactive force fields for the $SrFe_{O3}$, $SrCr_{O3}$ and $La_{0.3}Sr_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$ perovskite oxide-based electrodes.

Final remarks

- The developed reactive force field will allow Irfan to understand the degradation mechanism of the perovskite's electrode under various conditions.
- The developed reactive force field will enable understanding of the electrocatalytic CO_2 reduction reaction mechanism as well as other electrocatalytic oxidation and reduction reaction mechanisms on the $La_{0.3}Sr_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$ perovskite-based electrode surface.

Advanced electrochemical system for energy storage through CO_2 conversion

In operando XAS investigation of CO_2 reduction in perovskite-based reversible solid oxide cells

Oliver Calderon
PhD student

Introduction

Oliver Calderon studies perovskite materials that catalyze the reduction of CO_2, which would allow the removal of carbon emissions from the atmosphere. These materials are efficient, selective and contain earth-abundant metals. His project revolves around using extremely brilliant X-rays produced by the synchrotron at the Canadian Light Source (CLS) to probe the mechanism of this reaction.

The insights from observing the breakdown of CO_2 in real time will lead to better design of CO_2 electrocatalysts — enabling such devices to be cheaper and more ubiquitous. This technology is the potential backbone of the sustainable, zero-emission energy system that humanity needs.

Results

This challenging project brings together synthesis, design, engineering, device fabrication, electrochemistry and advanced characterization techniques. Oliver has synthesized a wide range of perovskite materials which vary in their calcium, strontium and chromium content. Using these materials, he has begun to manufacture electrochemical cells that can be used with electrochemical testing to study the effect of element doping on their CO_2 electrolysis efficiency. Eventually these cells will be brought to the synchrotron and subjected to in operando X-ray absorption studies; these experiments will observe CO_2 reduction as it occurs at the surface of fully operating electrolysis devices in real time. Oliver has designed and begun prototyping a special apparatus that will permit in operando studies — a major component of his research project. In addition, Oliver has worked with collaborators to corroborate their computational studies of CO_2 reduction on perovskites. His experimental results will be included in a manuscript to be submitted soon.

Final remarks

- The potential impact of this project is immense and could lead towards a truly closed-loop energy system.
- Important preliminary X-ray absorption experiments have been completed at the Canadian Light Source — including in situ work that is a stepping stone to the ultimate goal of in operando research.
- Significant progress has been made on all synthetic, characterization and apparatus milestones.
- Work has also progressed on several exciting studies that are expected to provide novel insight into the effect of element doping and surface area on CO_2 electrocatalysts.

Advanced electrochemical system for energy storage through CO_2 conversion

Mykhailo Pidburtnyi
PhD student

Introduction

Newly developed metal oxide-based catalysts for solid oxide electrolysis cell (SOEC) and solid oxide fuel cell (SOFC) applications allow significantly improved carbon dioxide to carbon monoxide conversion rates, thus making the technology more efficient. However, to allow rigorous comparison with other catalysts, it is critical to determine the activity at a known surface area. This is being done by using pulsed layer deposition (PLD) to produce smooth, pore-free $La_{0.3}M_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$ (LMFCr) films, although it has been shown that the current collector used must be inert in the CO_2 environment. In another direction, other properties of LMFCr are being determined (e.g., conductivity) through various collaborations. Work is also underway to investigate the activity and stability of LMFCr in steam/CO_2 mixtures, allowing the production of tunable syngas (H_2+CO).

Results

Atomic layer deposition-produced LCFCr thin films were obtained from University of Alberta, and the smoothness and film composition were determined, showing a root mean square (RMS) roughness of 0.2-0.5 nanometres and uniform distribution of elements within the whole film, although the film thickness was less than desired (25 nanometres instead of 100 nanometres). Even so, when electrochemically tested, it was found that the current collectors must be as inactive as possible so that they do not contribute to the measured activity of the smooth (low area) LCFCr material. To determine their activity in CO_2 gases and in air, porous platinum (Pt) and gold (Au) composite electrodes were produced using infiltration methods and the electrochemical activity was determined. The results showed that in air, Au is eight times less active than Pt. Similarly, in CO_2, Au is 70 times less active than Pt. As Au is much more inert in both environments, it is the preferred material for use as the current collector in thin films studies.

Final remarks

- Gold is the preferred current collector material for the study of the catalytic activity per real area of LMFCr thin films towards CO_2 reduction.
- As this work was carried out with a zirconia-based material in contact with Au or Pt, future work will be conducted to determine the activity of Au and Pt contact to the LMFCr catalyst material itself.
- The infiltration technique used in recent work can be further used to produce high-surface area electrodes.
- The catalytic properties of the LMFCr perovskite are currently being determined by the electrical conductivity relaxation technique in various gas environments, which is expected to be critical to the LMFCr catalyst properties.
- The new setup for syngas production through steam/CO_2 co-electrolysis is currently being constructed.

THERMAL IMPACTS FOR GEOLOGICAL STORAGE OF CO_2

UCalgary Team: **Don Lawton**, Steven Bryant, Bernhard Mayer, Kristopher Innanen, Hassan Hassanzadeh

UAlberta Team: **Rick Chalaturnyk,** Ben Rostron

Background

Carbon capture and storage (CCS) is a key technology to enable Canada to meet its 2030 greenhouse gas (GHG) emissions reductions targets. A key big research question is to assess the capacity of subsurface formations to receive and safely store CO_2 over long periods of time and to support the regulatory framework of CCS and to alleviate any public concerns about this technology.

Research strategy

To address this question, collaborative research is being undertaken into modelling multiphase flow, heat transport and geomechanical changes that may occur due to CO_2 sequestration. The injected CO_2 will be at a different temperature than the target formation, in liquid or gas state at different depths and will be less dense than the aquifer water so that the injected CO_2 may migrate due to density and pressure gradients. Wellbore integrity can also be affected by temperature fluctuations within the nearfield environment of the well. It will vary with the heat transferred from the fluids flowing in the well. This project presents the opportunity both to validate an existing physical model with real field data and to better constrain heat transfer predictions between the wellbore and the near well environment. The research will also improve on the existing understanding of various thermal issues related to CO_2 sequestration, including injectivity index and downhole injection temperature, CO_2 phase behavior, density mixing, changes in formation porosity and permeability, deformation of the geological Storage Complex and risk of leakage.

Desired outcomes

The current research will shed light, for the first time, on the significance of thermal impacts on CO_2 storage operations. There will be better understanding of storage complex attributes that impact CO_2 injectivity and the security of CO_2 storage. The project team will be able to quantify the role of thermal issues in surveillance technologies applied to assess containment and conformance. The intent is to accelerate secure geological storage of CO_2 as an important GHG emissions reduction strategy.

Thermal impacts for geological storage of CO_2

Time-lapse elastic imaging for CO_2 monitoring using distributed acoustic sensing

Jorge Enrique Monsegny Parra
PhD Student

Introduction

Jorge Enrique Monsegny Parra aims to explore the feasibility and quality of different elastic imaging techniques, mainly elastic reverse time migration (RTM) and elastic least squares reverse time migration (LSRTM), for CO_2 monitoring with distributed acoustic sensing (DAS) data with a baseline and numerous monitor surveys. For this research, he is using DAS vertical seismic profile (VSP) data from the Containment and Monitoring Institute (CaMI) Field Research Station (FRS) at Brooks, Alberta.

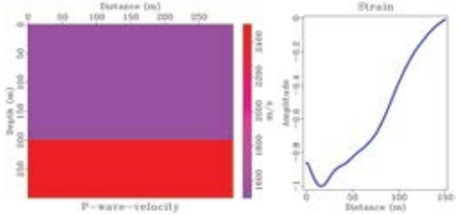


Figure 1

Results

Jorge has been working on a special imaging condition related to elastic strain that can be used with DAS data and will be the central part of the RTM and LSRTM techniques that will be used for CO_2 monitoring. The central part of this imaging condition is a version of the acoustic coupled finite difference wave equation system in pressure and particle velocity that is modified to propagate normal strains. As DAS data is usually strain or strain rate, imaging with this system is more natural than transforming DAS to pressure. Figure 1 displays a two-layer synthetic model and the strain response at the interface between the two layers after RTM. Figure 2 shows the result of using this imaging condition in the vertical seismic profile of data from CaMI-FRS.

Final remarks

- The strain imaging condition is a more natural imaging condition to image DAS data than transforming this DAS data to particle velocity and then imaging.
- The response of the strain imaging condition along the interface in the synthetic model shows a curve very similar to the usual response obtained from geophone data.
- The RTM using the strain imaging condition in the DAS VSP data from CaMI-FRS shows a good balance of amplitudes from all reflectors and is comparable to the geophone result.

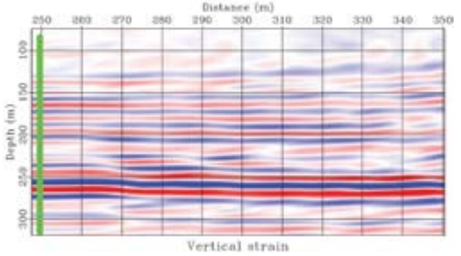


Figure 2

UNLOCKING THE PHYSICS AND CHEMISTRY OF BITUMEN/WATER/SOLVENT/POROUS MEDIA INTERFACES — AN ENABLING TECHNOLOGY FOR NEW PRODUCTION PROCESS DEVELOPMENT

UCalgary Team: **Apostolos Kantzas**, Harvey Yarranton, Ian Gates, Giovanniantonio Natale

UAlberta Team: **Juliana Leung**, Hongbo Zeng, Japan Trivedi, John Shaw

Background

As a result of significant challenges faced by the oil sands industry, the focus will and should be on developing and applying new technology to improve the effectiveness of ongoing sub-surface operations. Improvements to ultimate recoveries from reservoirs, improvement in energy efficiency (i.e., reduced steam-oil-ratio) in heterogeneous reservoirs and the ability to access the parts of current producing fields that have production challenges such as top gas and bottom water. New insights into these problems will allow for extension and improvement of existing thermal operations, provide access to top gas/bottom water zones that are currently second tier resources and promote the development of next-generation production technologies with significantly lower environmental impacts.

Research strategy

The contribution of the project team will focus on pore scale bitumen/water/solvent interfaces and bitumen/water/chemical interfaces and their evolution during solvent, thermal, thermal-chemical and thermal-solvent production processes. The team's major goal is to resolve the physics/chemistry of these interfaces within porous media. The first line of inquiry will focus on studying the interfaces in bitumen/water/solvent systems with the goal of understanding how solvent contacts oil in the presence of water and how changes in oil composition can affect solvent mass transfer and retention in porous media. This will build on the insights gained regarding interfacial responses and mechanisms for movement of water/bitumen/solvent mixtures within porous media.

Desired outcomes

This research will result in an improved understanding of interfacial dynamics that will permit design of new solvent packages that will yield significant reductions of greenhouse gas (GHG) intensity, improvements to energy efficiency, and offer the joint aspects of greater production rates and ultimate recoveries. The project team will have experimental data and models related to the use of electromagnetic and acoustic excitation intended to improve the access and hence the effectiveness of solvents and foams in porous media in both existing and emerging bitumen production process technologies.

Unlocking the physics and chemistry of bitumen/water/solvent/porous media interfaces — an enabling technology for new production process development

Investigating acoustic levitation for processing liquids

Lyndon Bunio
MSc student

Introduction

Levitation of liquid drops enables contactless processing of liquids — this can enable reaction and conversion technologies that are not possible in traditional reaction chambers and vessels. This project is examining the levitation of water droplets to understand its dynamics and design of equipment used for levitating droplets. The initial work has been on evaporation of liquid droplets (water, alkanes, alcohols) with comparisons to theory.

Figure 1

Results

The results of the research demonstrate that levitation of droplets is possible and that the droplets can be held in space for extended periods of time. For processing liquids in contactless levitation reactors, due to acoustic streaming, the droplets will evaporate given sufficient time. This time depends on the droplet diameter, air temperature and humidity, and composition of the droplet. The experimental results confirm theoretical predictions. The theory can be extended to model crystallization of solids within levitated evaporating droplets.

Final remarks

- The evaporation rate of levitated droplets depends on air temperature, humidity and initial droplet size.
- Droplets can be controlled in space to within a few millimetres and can be moved in space via alterations to the acoustic field.
- A theoretical model has been derived which is capable of predicting the evaporation behaviour of levitated droplets.

Unlocking the physics and chemistry of bitumen/water/solvent/porous media interfaces — an enabling technology for new production process development

Amir Fayazi
Postdoctoral Fellow

Introduction

Improving flow and transport in porous media is of concern for many practical applications including remediation of groundwater contamination, enhancing oil recovery, CO_2 sequestration and enhancing chemical reactions. Experimental, analytical and numerical investigations, as well as some pilot and field studies, have shown that propagation of acoustic waves can enhance flow and transport in porous media. Acoustic excitation with different frequencies is transferred by the mechanical waves which can propagate through solid, liquid and gases with different velocities. The use of sonic energy provides an economically-feasible and environmentally-friendly alternative to facilitate oil recovery and groundwater remediation.

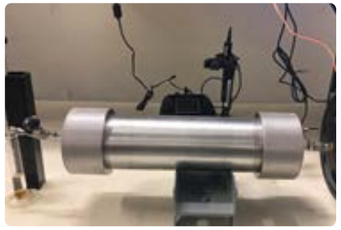


Figure 1

Results

Dr. Amir Fayazi, PhD, designed a flow apparatus with a special housing for an actuator to directly vibrate the injected fluids with different frequencies and amplitudes in miscible/immiscible displacements inside confined porous media (Figure 1). Various fluids were injected into a water-saturated porous medium, with and without the acoustic field to demonstrate how mechanical excitation can influence the fluid flow in porous media. Effluent fluids were captured as a function of time and were used to calculate the efficiency of the acoustically-assisted displacements.

Amir also developed a pore-scale model to study the influence of acoustic excitation on dispersion in porous media. The modelling involves first solving fluid flow without the acoustic field, then calculating an external acoustic pressure field across a saturated medium containing a stationary fluid, and finally evaluating the interaction between the acoustic field and the flowing fluid.

Final remarks

- In simulations, temporary velocity variations created by propagated waves enhanced the dispersion process during miscible displacement.
- In simulations, lower frequencies and higher acceleration amplitudes of the propagated waves increased the dispersion enhancement by providing a longer half-cycle wave for continuous excitation and creating larger local velocity variations.
- Immiscible and miscible experimental tests are under process.

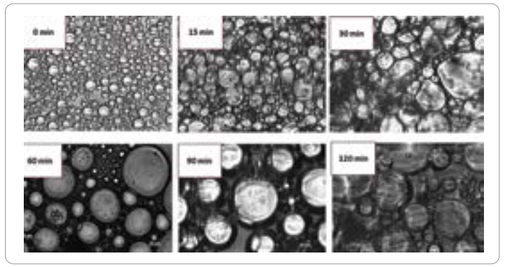
Unlocking the physics and chemistry of bitumen/water/solvent/porous media interfaces — an enabling technology for new production process development

Acoustic excitation of asphaltene stabilized water/model oil emulsion

Razie Khalesi Moghaddam
PhD student

Introduction

Razie Khalesi Moghaddam aims to clarify the exact mechanism of destabilization of water/oil (W/O) emulsions. She will do this using ultrasound and interfacial rheology (dilatational and microrheology). She is trying to develop a novel microrheology method to characterize asphaltene-laden interfaces. Her goal is to find a framework for destabilizing W/O emulsions in terms of ultrasound field features.



Results

Razie determined the dilatational rheology of asphaltene-laden W/O interfaces in the static mode. She showed that ultrasound can destabilize asphaltene water/model oil emulsions very fast. To achieve this, she built a home-made setup to perform interfacial microrheology. She characterized the W/O interfaces by using different fractions of asphaltenes.

Final remarks

- Ultrasound waves can promote coalescence in the asphaltene stabilized water/model oil emulsions due to higher frequency of the collision between drops and weakening of the asphaltenic interface.
- Asphaltene fraction which has a higher number of polar groups is responsible for stabilizing the W/O emulsions.
- The interfacial rheological characteristics of the fraction having higher number of polar groups, are significantly higher than other fractions.

Unlocking the physics and chemistry of bitumen/water/solvent/porous media interfaces — an enabling technology for new production process development

The excitation of fluid displacements in porous media using acoustic waves

Saeid Khasi
PhD student

Introduction

Enhancing processes of flow and transport in porous media is of concern for many practical applications, including enhancing oil recovery, remediation of groundwater contamination, geological carbon dioxide sequestration and enhancing chemical reactions. Experimental, analytical and numerical investigations, as well as some pilot and field studies, have shown that propagation of acoustic waves can enhance these processes.

The objective of Saied Khasi's study is to investigate whether and how acoustic excitation/stimulation can improve flow and transport during miscible and immiscible displacements in porous media. In this study, he will develop pore-scale and continuum models, and perform micromodel and sand pack experiments.

Results

Saied developed a pore-scale model to study the influence of acoustic excitation on dispersion during miscible displacement in porous media. The model was implemented on a pore-scale heterogeneous porous medium, which is constructed based on a simplified image of a real medium. Using simulation results of the developed model, the effects of controlling parameters, including background velocity field, acoustic frequency and amplitude were investigated. These results were summarized in a proposed dimensionless group for designing effective acoustically-assisted experiments in the laboratory. The results of this work provide a better understanding of the beneficial mechanisms of acoustic stimulation and can be used in future experimental designs that aim to investigate the practical effect of acoustic excitation on miscible displacement.

Final remarks

- Oscillations of acoustic waves could change the holdup transport regime by locally breaking up the closed streamlines in the velocity field and decreasing stagnant volume effects in a miscible displacement.
- In addition to changing the holdup dispersion regime, mechanical dispersion can be improved in acoustically-assisted displacements due to the additional average velocity attributed to acoustic waves.
- Lower frequencies and higher acceleration amplitudes of the propagated waves increase the ratio of the dispersion enhancement.
- Simulation results for displacing viscous fluids indicate that low-frequency excitation could be a promising technique for improving heavy oil recovery by changing the dispersion regime in a miscible displacement.
- There are beneficial mechanisms in acoustic excitation in miscible displacement.
- Saied's next step is investigating possible mechanisms in immiscible displacements. Both miscible and immiscible experiments will be performed to verify the simulation results and study the feasibility of using acoustic energy for recovery enhancement.

RESERVOIR MANAGEMENT AND ADVANCED OPTIMIZATION FOR THERMAL AND THERMAL-SOLVENT BASED RECOVERY PROCESSES USING FUNDAMENTALS, SCALED MODELS AND MACHINE LEARNING

UCalgary Team: **Ian Gates,** Hossein Hejazi

UAlberta Team: **Japan Trivedi,** Juliana Leung

Background

Steam-assisted oil recovery methods such as steam-assisted gravity drainage (SAGD), expanding solvent steam-assisted gravity drainage (ES-SAGD) and cyclic steam stimulation have been successfully applied in the oil sands, however, these require a significant amount of steam. Optimization at every scale, including fundamental studies, scale-up processes and reservoir management, is essential for low-cost and energy-efficient thermal process developments.

Research strategy

The approach is to perform mechanistic small-scale high-resolution simulations, where detailed heterogeneities at the fine scale are explicitly represented — the goal being to model directly how solvents would propagate to/across/away from the interface and into the oil. A robust optimization workflow will be developed that optimizes various operational parameters of the thermal recovery processes in the presence of various uncertainties (such as geological and geomechanical uncertainty). In addition, the stochastic nature of distinct fundamental physical phenomena (e.g., molecular diffusion in solvent processes) will also be incorporated in the proposed optimization workflow using scaled models. Big data analytics will be utilized to examine the abundant data available from the day-to-day field operations, which can potentially uncover the hidden trends and unknown correlations and predict the short-term and long-term reservoir behavior. This behavior coupled with scaled models or by themselves can be used for quick real-time optimization and decision-making.

Desired outcomes

This research will reduce steam requirements and maximize recovery for various thermal processes, thus improving significantly the emissions intensity and energy efficiency of the recovery processes. Real-time decision-making for optimization to improve existing operations and reduce emissions and water use will also be possible. Additionally, new mathematical models will be developed to enable rigorous and robust optimization of recovery process design. Finally, the life cycle of existing thermal operations within the framework of automated optimization of recovery operations will be extended.

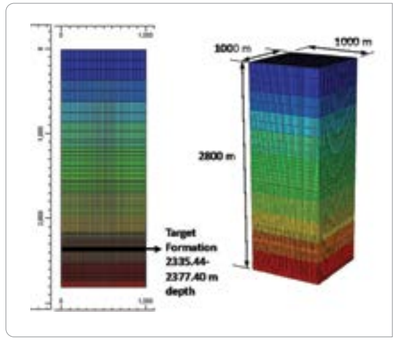
Reservoir management and advanced optimization for thermal and thermal-solvent based recovery processes using fundamentals, scaled models and machine learning

On energy extraction from a geothermal resource in central Alberta, Canada

Qinwan Chong
PhD student

Introduction

By the end of their economic life, thermal oil sands recovery processes leave behind roughly 70 per cent of the total injected heat within the reservoir. There is potential that some fraction of this remaining energy in the reservoir could be recovered using geothermal methods. In this research, geothermal simulation models are being constructed for the extraction of heat from both traditional geothermal sources and post steam-assisted gravity drainage (SAGD) operations. The operations will be optimized to maximize the energy return on energy invested from the hot rock source.



Results

Qinwan Chong has constructed a detailed earth model to assess energy return on energy invested for a candidate geothermal reservoir in Alberta. The geological model was based on well log data. Heat losses along injection and production wells are taken into account. From detailed geological modelling and thermal reservoir simulation, different well configurations were studied. The results show that the energy return to energy invested ratio ranges from low (1 gigajoule return per gigajoule invested) to high (12 gigajoules return per gigajoule invested) depending on the well configuration, operating rate and permeability of the reservoir.

Final remarks

- The geothermal formation's permeability can limit the production of water from the reservoir under certain well configurations.
- Practical well configurations and operating conditions can be realized with sufficiently high energy return on energy invested.
- Geothermal development in Alberta will require careful design and operating strategy to yield useful energy returns.

Reservoir management and advanced optimization for thermal and thermal-solvent based recovery processes using fundamentals, scaled models and machine learning

Fishbone well architecture improves SAGD performance in complex reservoirs — Surmont field SAGD enhancement

Benjamin Edafiaga
PhD student

Introduction

This project aims to achieve improved oil sands recovery process performance beyond that of conventional steam-assisted gravity drainage (SAGD) in complex reservoirs by adding fishbone multilateral wells and flow control devices (FCDs) on both injectors and producers. The goal is to develop new recovery process designs that yield improved bitumen recovery, improved net present value (NPV), reduced cumulative steam-oil ratio (cSOR) and reduced greenhouse gas (GHG) emissions, hence improving the overall efficiency of the SAGD process.

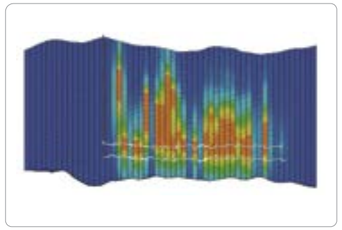


Figure 1

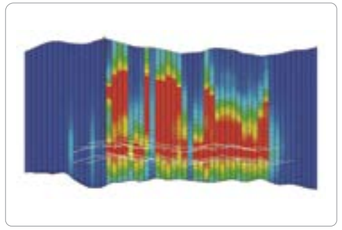


Figure 2

Results

In this research work, Benjamin Edafiaga developed a fishbone well architecture/model to improve SAGD performance beyond the near wellbore for complex reservoirs. Doing that was hitherto difficult due to the complexities of the reservoir, different facies in the reservoir and the silt/shale lateral reservoir arrangements that impede steam flow, thereby reducing steam chamber conformance. The introduction of the fishbone well architecture combined with FCDs improves production from such complex reservoirs by approximately 60 per cent.

Final remarks

- The results demonstrate that the fishbone well architecture installed on injector and producer wells increases the production rate and ultimate recovery from complex reservoirs over that of standard SAGD.
- The reduction of the steam-to-oil ratio implies that the environmental impact of the recovery process is reduced.
- The fishbone laterals crisscross shale barriers to access sections of the reservoir rich with bitumen, thus increasing long-term productivity in heterogenous and complex reservoirs with severe heterogeneity.

MONITORING THE STRUCTURAL RESPONSE OF STORAGE STRUCTURES TO CO_2 INJECTION — EXPLORING THE POTENTIAL OF PASSIVE SEISMIC MONITORING

UCalgary Team: **Hersh Gilbert**, Kristopher Innanen

UAlberta Team: **Jeffrey Gu,** Mauricio Sacchi

Background

Recent developments in seismic interferometry have led to successful extraction of body and surface waves from the ambient noise field to detect structures at CO_2 injection sites. These arrivals exhibit similar patterns to those produced by active seismic imaging in the same location, which underscore their potential for monitoring purposes. However, ambiguities in the images from these studies presented challenges in reproducing reliable and repeatable observations at the scale of storage structures at injection sites, or for detecting temporal changes in structures.

Research strategy

This research proposes to expand upon on these results through a collaborative project that includes collecting a novel passive seismic (PS) dataset at the Containment and Monitoring Institute (CaMI) Field Research Site (FRS), which is an active CO_2 injection site. A number of active sources will be generated at permanent positions to ensure consistency of the source at different times. These observations from active signals will serve as a reference to gauge the capabilities of passive monitoring and identify whether both datasets detect the same structural features. Also, sampling a larger area will illuminate the extent of the structures and the ground motion response to injection within the FRS. Knowledge gained from Phase 1 regarding the strengths and weaknesses of the initial dataset for PS analysis will be used to adjust and augment the array design of Phase 2.

Desired outcomes

By utilizing techniques normally employed for the analysis of active source data, this project will explore the potential of PS data to monitor CO_2 injection sites and what can be done to maximize its capabilities. The design of this project will facilitate the detection of temporal variations in structures over time periods within each three-month recording interval and between the two separate recording phases. Also, the structural examination that will come from this project will improve understanding of the response of reservoir formations to CO_2 injection.

Monitoring the structural response of storage structures to CO_2 injection — exploring the potential of passive seismic monitoring

Laleh Khadangi
PhD student

Introduction

Reducing greenhouse gases requires safe CO_2 sequestration. Seismic monitoring using controlled sources has typically been used to ensure safe CO_2 storage. A drawback of this approach is the need for man-made seismic sources, and that temporal changes in the storage formation would go unnoticed between surveys. Laleh Khadangi is developing monitoring approaches that use ambient seismic noise. Ambient seismic noise contains signals from the atmosphere, ocean waves, distant earthquakes and other anthropogenic sources, and can be used to investigate the subsurface structure. She will evaluate ambient noise monitoring approaches of CO_2 sequestration at the Containment and Monitoring Institute (CaMI) Field Research Station (FRS).

Results

The horizontal to vertical spectral ratio (HVSR) of the seismic time series has been shown to be sensitive to the shallow structure beneath a three-component seismic sensor. To implement this, Laleh has participated in collecting a new continuous passive-seismic database comprised of over 200 three-component sensors configured in a one-by-one kilometre array at the CaMI-FRS near Brooks, Alberta. By calculating the Fourier transform of both the horizontal and vertical signals, the HVSR curve can be determined. Using the HVSR curves, she evaluates the resonance frequency and amplification factor at each sensor. Generally, there are peaks at 20 and 2.5 hertz. The curves, and their peak frequencies, change between observations produced from data recorded during the day and night. The peak at 20 hertz appears sharper with higher values at night, shown in Figure 1, and the one near 2.5 hertz has higher amplitudes during the day, shown in Figure 2.

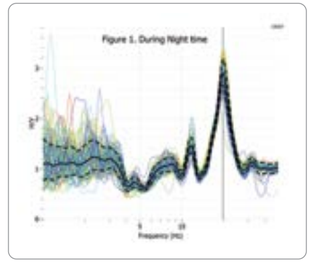


Figure 1

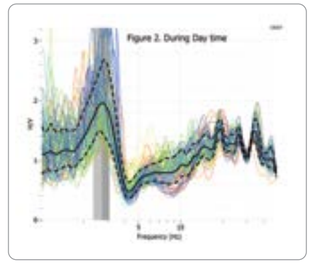


Figure 2

Final remarks

- HVSR curves show spectral peaks at 2.5 and 20 hertz. The peak frequencies represent the resonance frequency of the soil which is tied with soil properties.
- The HVSR value exhibits an amplification factor for the site which is not stable for the peaks observed during either the day or night.
- The observed differences between the spectral signal observed in the day and night likely result from the seismic data being noisier during the day.

Monitoring the structural response of storage structures to CO_2 injection — exploring the potential of passive seismic monitoring

Genevieve Savard
Postdoctoral Fellow

Introduction

The Containment and Monitoring Institute (CaMI) Field Research Station (FRS) is a laboratory to test and refine monitoring technologies for the early detection of CO_2 leakages. Dr. Genevieve Savard, PhD, explores the potential of various passive seismic monitoring techniques including detection and characterization of induced microseismicity, ambient noise correlation and Green's function methods to potentially track stress perturbations, fluid movement and composition (velocity) perturbations caused by the CO_2 and pressure plumes.

Results

The geophone arrays used for passive seismic monitoring require monthly visits to the FRS for replacement and data retrieval. After format conversion and signal pre-processing, Genevieve analyzes the waveform records using a variety of methods to detect microseismicity and long-period long-duration signals. These events are then characterized in terms of location, magnitude and source mechanism. The onset of induced microseismicity shows interesting patterns: shallow depths, above the reservoir and correlation with bottom well pressure. The low magnitudes require advanced inversion techniques to extract source mechanisms. Long-period long-duration signals are intriguing events that are being studied. Probabilistic inversions using distant teleseisms have also shown promise for resolving deep sedimentary velocity structure and possibly perturbations in velocity due to CO_2 injection.

Final remarks

- The CaMI-FRS is a shallow injection site that presents a unique opportunity to understand the seismic signature of shallow CO_2 injection or leakages.
- Induced-microseismic activity has started at the FRS in January 2020 and many interesting patterns are currently being studied.
- Waveforms of distant teleseisms and ambient noise recorded by the dense geophone arrays can also be used to invert for velocity structure and perturbations in time due to injection of CO_2.

ASSESSING POLITICAL PATHWAYS FOR ENERGY TRANSITION

UCalgary team: **Melanee Thomas**

UAlberta team: **Lori Thorlakson**

Background

The goal of this research project is to assess the political viability of policies that support the transition to low-carbon energy strategies, including the explicit phasing out of high greenhouse gas (GHG) emitting energy generation. Yet, democratic politics, public opinion, federalism and Indigenous rights may all constrain the reliance on scientific evidence and adoption of technical innovation, so that while a low-carbon economy may be technically feasible, it could be/is thus far politically impossible.

Research strategy

This project has three phases: (1) The research group has to assess how public opinion about energy transition is formed and shaped, focusing on the effects of ideology, populism, cynicism and Indigenous rights claims. Here, the group uses the Alberta Narratives Project as a base. The Alberta Narratives Project is a large-scale qualitative research project on energy transition communication that brings together industry stakeholders, civil society and government to identify how various messages regarding energy transition impact audiences in different ways. Survey experiments show the effectiveness of these narratives across Canada. (2) Using these results, they will investigate which factors, such as public opinion, Indigenous rights and scientific entrepreneurship, policymakers consider when drafting policy and regulations about energy transition. (3) The research team will ask how federalism and multi-level governance affects when and how government adopts energy innovation.

Desired outcomes

Climate change is an acute problem. Understanding how the public reacts to energy transition policy will be of paramount importance. The adoption of these policies is less a question of if and more a question of when. Racism towards Indigenous peoples is also an acute problem. Indigenous consent may be mandatory for projects to go forward; thus, understanding settler reactions to Indigenous peoples exercising their rights is crucially important. Comprehending the importance government and politicians place on this public opinion is crucial to understanding when energy transition, and its corresponding technology, become politically viable options.

Assessing political pathways for energy transition

Brooks DeCillia
Postdoctoral Fellow

Introduction

The aim of this project is to identify the key drivers of public support of and opposition to energy innovation and climate policy using panel studies and survey experiments, and test which narratives on energy innovation and climate policy are the most persuasive. Through this, Dr. Brooks DeCillia, PhD, will identify how energy policy becomes salient for, and is supported by, both the public and policy makers.

Results

Brooks and his research team piloted a survey instrument in Alberta to test how energy narratives identified through a large-scale qualitative study of industry, civil society and government (led by an external collaborator) are affected by a range of attitudinal and demographic factors (such as trust, optimism, partisanship, economic role identifications, age and gender). He plans to conduct follow-up panel studies covering four Canadian provinces that represent a range of carbon pricing policies. This allows him to test hypotheses in the literature about the dynamics of public support for carbon pricing with intervening provincial elections in which carbon pricing is likely to be an important campaign theme.

The first phase of this research has been presented at two academic conferences. A paper is forthcoming.

Final remarks

Support for energy transition is shaped by:

- Social background.
- Underlying values, beliefs and other social orientations.
- Climate and energy perspectives and identities.
- New media.

LOW-COST CATALYSTS AND METHODOLOGIES FOR PARTIAL UPGRADING OF BITUMEN

UCalgary team: **Josephine Hill**, Jinguang Hu

UAlberta team: **Jeffrey Stryker**, Samir Mushrif, Natalia Semagina

Background

For the oil sands industry, the big question is, “Can minesite and in situ bitumen be transformed for transport without dilution by large volumes of solvent and without the high costs associated with complete upgrading into synthetic crude oil?” For the near term, this question has elicited the concept of “partial upgrading”. Less a process than economic proposition, there is no consensus on what partial upgrading entails, much less how, operationally, to accomplish it. In this collaborative program, it is proposed to address the question of whether inexpensive catalysts can be developed that partially and selectively hydrogenate aromatic systems in bitumen, reducing both viscosity and density to meet or exceed pipeline specifications.

Research strategy

The strategy includes development of catalysts for viscosity reduction via deaggregation of asphaltenes by chemical transformation, direct bitumen-to-liquid-crude conversion through catalytic thermolysis under mild conditions, and selective catalytic hydrotreatment at the distribution hub, on the minesite, or in situ. This research is using purpose-driven catalyst design with the support of theoretical and computational calculations to create bitumen-derived carbon-based catalysts.

Desired outcomes

Innovations in science, including (1) the development and demonstration of new concepts in catalyst design, molecular and nanoscale, and (2) new process technology adapted to the requirement for mild, energy-efficient reaction conditions, unprecedented for bitumen processing.

Low-cost catalysts and methodologies for partial upgrading of bitumen

Ana Cristina Baffa Carlotto
MSc student

Introduction

Ana Cristina Baffa Carlotto has been investigating how different ball milling parameters impact the surface of petroleum coke (petcoke). The goal is the conversion of the petcoke into catalysts for the partial upgradation of bitumen. This study contemplates the fundamental properties of petcoke and how they are affected by ball milling by comparing petcoke with different carbon species such as biochar. The relevant properties of a dispersive catalyst for bitumen upgrading reactions are also investigated.

Results

Ana has tested different petcoke milling conditions in the presence and absence of solvents. She has concluded that wet milling results in a higher homogeneity of the particle sizes. Dry ball milling conditions resulted in a wider particle size distribution (blue curve). The scanning electron microscopy (SEM) was one of the main techniques used, supported by Fourier-transform infrared spectroscopy (FTIR) and Boehm titration. Figure 1 shows the SEM image before and after dry milling, and the particle size reduction succeeding the milling process is visible. Ball milling is shown as a promising technique for reducing particle size of powder materials and for preparing dispersive catalysts. However, it was observed that only ball milling petcoke is not enough to create new surface groups on petroleum coke. The higher surface area can be developed in the wet milling as presented in the Figure 2 scheme.

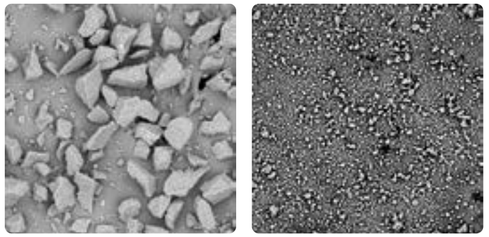


Figure 1

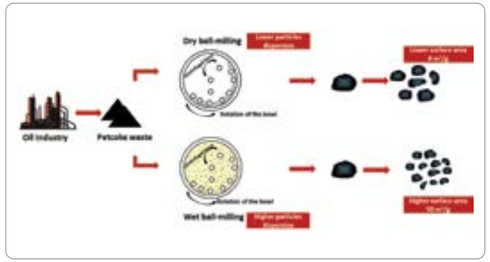


Figure 2

Final remarks

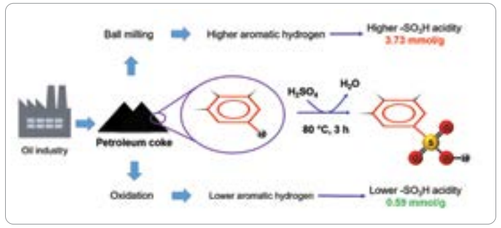
- Ana concluded that milling can significantly reduce the particle size of petcoke. However, new surface groups are not created in the milling process in the presence or absence of a solvent.
- Total acidity does not change significantly after ball milling.
- Wet ball milling results in more homogeneity and smaller petcoke particle sizes. Wet milling resulted in a higher surface area compared to dry ball milling (50 square metre per gram versus 8 square metre per gram).

Low-cost catalysts and methodologies for partial upgrading of bitumen

Ye Xiao
Postdoctoral Fellow

Introduction

Dr. Ye Xiao, PhD, aims to convert petroleum coke (petcoke), a by-product of the oil sands industry, into catalysts that can be used in the energy sector. Petcoke is usually stockpiled on site, taking up extensive land area and contributing to air pollution. The applications of petcoke, however, are limited due to its high sulphur content (up to approximately seven weight per cent). In this project, Ye demonstrates that petcoke can be converted to different types of catalysts including solid acid catalysts, which can esterify organic acids with methanol to generate components of biodiesel. Other catalyst formulations and heavy oil/bitumen applications are currently being explored.



Results

In this study, sulfonation of petcoke by concentrated sulphuric acid was carried out to produce solid acid catalysts. After sulphonation at 80 C for three hours, sulphonic acid (SO_3H) was successfully added to the petcoke samples. A SO_3H acidity of 1.25 millimoles per gram was obtained for raw petcoke (45-90 micrometres). If the petcoke was oxidized before sulphonation, hydrogen was removed and the resulting acidity reduced to 0.59 millimoles per gram. If the particle size was reduced by ball milling before sulphonation, more aromatic hydrogen was accessible and the resulting acidity increased up to 3.73 millimoles per gram. The sulphonated petcoke catalysts were tested and found to be active for the esterification of octanoic acid at 60 C with turn over frequency (TOF) ranging from 48 to 85 h^{-1}. The results give insights into the preparation of solid acid catalysts from carbon materials and highlight the application of petcoke without activation as a feedstock for solid acid catalysts.

Final remarks

- Petcoke can be directly sulphonated under mild conditions without activation.
- An increase in sulphonic acid acidity correlates to an increase in aromatic hydrogen.
- Ball milling improves the acidity from 1.25 to 3.73 millimoles per gram.
- Prepared catalysts are active for esterification of octatonic acid with TOF of 48-85 h^{-1}.

TECHNION RESEARCH COLLABORATION

The University of Calgary has secured a partnership with Technion, the Israel Institute for Technology, by leveraging its world-class capacity in chemistry and chemical engineering. Together, collaboration in Material Science, Imaging and Catalysis is already underway and the two institutions are working together on innovation and discovery.

UCalgary and Technion will continue to facilitate technical workshops and interactions among researchers, exchange samples and data, create opportunities for co-supervision of graduate students and postdoctoral fellows and establish a visiting program for scholars to work together on joint projects.

University of Calgary faculty members involved in the projects in this section are Profs. Viola Birss, Steven Bryant, Ian Gates, Kunal Karan, Edward (Ted) Roberts, Venkataraman Thangadurai, Milana Trifkovic, Simon Trudel and Sathish Ponnurangam.

ENGINEERED INTERFACES FOR ADVANCED ENERGY MATERIALS

UCalgary Team: **Milana Trifkovic,** Steven Bryant

Technion Team: Ofer Manor, Tamar Segal-Peretz

Background

The aim of the project is to combine interfacial rheology and interparticle interactions to tune the kinetics of lamella and nanoparticle jamming at oil-water interfaces, control the rate of emulsion droplet coalescence and tailor the resulting mechanical properties of dense emulsions and bi-continuous fluids. This basis knowledge is applied in the design of nanostructured complex fluids — fluids that contain engineered nanoparticles, possibly along with chemicals, sometimes in one but most often in multiple phases — that will enhance oil recovery processes and also be applied for the development of advanced energy materials.

Research strategy

Here the project team investigates the microscale inter-particle interactions through a variety of microscopic techniques followed by confocal-rheology experiments. Photonic force microscopy (PFM) experiments allow the measurement of attractive interactions of individual droplets armored by particles, surfactants or both, which provides insight into the rheological behavior of the bulk emulsions. Laser scanning confocal microscopy (LSCM) visualization of complex fluid flow through a sand pack allows for an improved understanding of how oil displacement occurs during nanofluid or emulsions flooding of oil reservoirs for enhanced oil recovery. Finally, confocal-rheology experiments allow researchers to connect the microstructure of the derived complex fluids to their rheology and be able to tune them for the application of interest.

Outcomes

This project is creating new classes of complex fluids with tailored nanoparticles and developing novel imaging techniques that reveal how these fluids behave.

- This study has yielded an important discovery — anisotropic nanoparticles can form several micron long bridges between the droplets.
- Confocal-rheology instruments establish the correlation of complex fluid microstructure with functionalized cellulose nanocrystals (CNC) to their rheological properties.
- Preliminary coreflood experiments with cellulose nanocrystal-stabilized emulsions show promising results in terms of blocking the flow of oil and water until a threshold pressure gradient is applied.
- Methods for ex situ characterization of the developed emulsions systems using cryo-scanning electron microscopy (cryo-SEM), cryo-transmission electron microscopy (cryo-TEM) and inductively coupled plasma mass spectrometry spectroscopies (ICPMS) have been developed.

Engineered interfaces for advanced energy materials

Investigation of emulsion flow through porous media via micro-sandpack coupled with laser scanning confocal microscopy

Aigerim Meimanova

PhD student

Introduction

Aigerim Meimanova is developing a microscopic morphological complex-fluid behaviour correlation to a macroscopic response. The microscopic characterization is made possible by coupling a specially-designed micro-sandpack apparatus with confocal laser scanning microscopy. The macroscopic response is evaluated through differential pressure measurements across the whole length of flow. Emulsion droplets of the fluid used for the experiments have capabilities of interacting with each other, and these create complex behaviour during flow through the micro-sandpack. Currently, Aigerim is working on developing a model that ties the pore-scale emulsion behaviour to the generated pressure profiles and the structural evolution during flow.

Results

Aigerim has designed a micro-sandpack apparatus with high-pressure capabilities. The setup has been successfully tested to obtain visual insights to the pore-scale emulsion flow and external differential pressure measurements. During experiments, she has detected specific pore-scale events and corresponding pressure responses. The attractive potential of the nanoparticles used to stabilize the emulsion provides an additional trigger to emulsion destabilization or coarsening. Once the droplets pass the sand grain, they lose part of their external layer coverage during slow flow with prolonged contact time, which makes them prone to coalescence. Hence, the slow flow is characterized by changing emulsion morphology. In the contrary, during the fast flow, the high shears often result in new emulsion generation from the available phases in situ and lead to crowded pore throats and jamming, which in turn causes pressure to build up. The recurring pressure buildup and release cycles are explained through imaging insights.

Final remarks

- Aigerim detected the in situ events characteristic of each pressure buildup and release stages of constant emulsion injection flow.
- The early low-pressure flow shows distinct subsequent droplet and nanoparticles deposits that identify old flow pathways. This stage also results in droplet coalescence.
- The onset of the next pressure buildup is defined by large droplets straining the pore throats.
- The buildup stage has slow or no flow, and it is culminated when the pressure has reached a value of yield stress for the emulsion fluid within the pathway.
- Aigerim is planning to test the emulsion flow behaviour and corresponding pressure response in hydrophilic and hydrophobic sandpack.

BEIJING RESEARCH COLLABORATION

Through the Global Research Initiative in Sustainable Low Carbon Unconventional Resources (GRI), the University of Calgary has taken a leadership role in driving innovative research in unconventional oil and gas in China. Focused on collaborative research, education and training, the Beijing Research Site leverages the University of Calgary's world-class expertise in unconventional hydrocarbon resources (UHR) and technologies such as shale and tight gas and oil, coal-bed methane, heavy oil, oil-sands bitumen and gas hydrates. Located in the Kerui Group's offices in Beijing, the Beijing Research Site houses state-of-the-art equipment and over 4000 square meters of laboratories for research related to unconventional hydrocarbon resources. This collaboration in China has led to many joint publications and growing research partnerships with companies, universities and institutions in China.

University of Calgary faculty members involved in the projects in this section are Profs. Steven Bryant, Shengnan (Nancy) Chen, Zhangxing (John) Chen, David Eaton, Ian Gates, Hossein Hejazi, Haiping Huang, Kristopher Innanen, Steve Larter, Bernhard Mayer and Cathryn Ryan.

IMPROVED AND ALTERNATIVE ENERGY RECOVERY FROM PETROLEUM RESERVOIRS

Ian Gates, Steve Larter, Haiping Huang

Background

The research conducted in this project deals with improvements of energy recovery from petroleum and harvesting of energy, in alternate form, from underground systems. This could be in the form of petroleum or other energy vectors, or simply as heat. Further improvements to production from petroleum systems can be achieved if there is a better understanding of the deposition of oil and its geochemical compositional distributions in the reservoir.

Research strategy

In the area of improved petroleum recovery, the project team is examining the distribution of proppant in hydraulic fractures, the profiling of biodegraded oil composition in oil sands reservoirs and point bar systems, analysis of hydrogen generation reactions during in situ combustion and in situ gasification of heavy oil, and natural gas co-injection with steam into the reservoir as a means to improve the performance (energy efficiency, economics and environmental impact) of oil sands recovery processes. Other systems examined include production of heat from geothermal systems and how the understanding of thermal management for steam-based recovery processes can be used to improve energy recovery from geothermal systems. The project team also examines the use of redox active transition metals, or other species, as alternative energy carriers (instead of the hydrocarbons themselves), that can potentially be produced to the surface to produce a carbon-free energy source from heavy oil reservoirs. Lastly, the team creates reservoir models for simulation of redox active transport metal energy recovery processes from heavy oil reservoirs.

Desired outcomes

This project has led to new insights on the layout of proppant in fractures, oil composition in point bar reservoirs, in situ reactions and hydrogen generation in heavy oil reservoirs, and how natural gas injection can support improved recovery performance. The principal geological environments will be identified where transition metal mediated oxidation of crude oil may occur. Moreover, modelling and definition of the thermodynamics and thermochemistry of crude oil oxidation with transition metal oxidants under a variety of geological environments will be developed. Laboratory datasets of oil and bitumen before and after reactions will also be created in addition to the reaction kinetics under different shuttle systems.

Improved and alternative energy recovery from heavy oil reservoirs

Solids management in unconventional resource development

Guangyu Shi
PhD student

Introduction

Solids handling in unconventional resource development means interacting with dust which can be a major health issue. For example, proppant is used in hydraulic fracturing for holding induced fractures in the reservoir open. The proppant consists of sand with typical diameters between 50 and 300 microns and with handling and transport, a lot of dust can arise. Thus, given the potential for health issues, there is a need for dust suppression and to do it at low cost.

Results

Many types of dust suppression methods and materials have been evaluated including polymers, oils and water additives. The results of the research have shown that a practical and low-cost option for completely suppressing dust arising from sands is through the use of sugar solutions. A key benefit is that the sugar solutions need not be food quality and are benign to the environment.

Final remarks

- The results show that the concentration of sugar in the solution must be within a specific range — too little does not suppress the dust completely whereas too much consolidates the sand.
- Using low-concentration sugar solutions, dust can be suppressed by up to 97 per cent in sands.

Improved and alternative energy recovery from heavy oil reservoirs

Molecular geochemistry of the Paleogene petroleum system in the Dongying Depression, Bohai Bay Basin, East China

Qianru Wang
PhD student

Introduction

Qianru Wang's research aims to explore the contribution of source input from the Kongdian Formation, the third member (Es3) and the fourth member (Es4) of Shahejie Formation. She will be using integrated molecular geochemical characterization of crude oil and source rock samples to guide the hydrocarbon exploration at the discovered reservoirs in the Dongying Depression, Bohai Bay Basin. She is investigating the compositional heterogeneity, thermal maturity and secondary alterations (mixing, biodegradation, thermal cracking) of the reservoir oils.

Results

Qianru has finished the petroleum geochemical analysis in the laboratory using a gas chromatograph coupled to a mass spectrometer. Data interpretation is currently under investigation. She has completed the oil-oil and oil-source correlation in the Dongying Depression. Novel parameters derived from alkylbiphenyls and alkyldiphenylmethanes have been proposed to assess the thermal maturity of sediments, and these results have been published in *Energy & Fuels.* The secondary alterations of reservoir oils, such as mixing and biodegradation, and their paleo-depositional environments have been quantitively investigated using a series of biomarkers.

Final remarks

- Oil mixing was common in the Dongying Depression and some "immature oils" were mixtures of early generated oils and later matured oils.
- Various degrees of biodegradation occurred in the oils from the Shahejie Formation in relatively shallower burial depth.
- Molecular concentration should be taken into account to assess the thermal maturity of reservoir oils.
- Source rocks in the Es4 member with abundant beta-carotene and phytane were deposited in more saline conditions than those in the Es3 member.

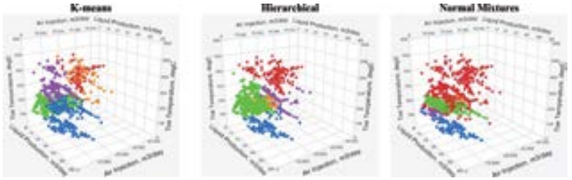
Improved and alternative energy recovery from heavy oil reservoirs

Data analytics of Kerrobert THAI project

Wei Wei
PhD student

Introduction

Wei Wei's research consists of a detailed analysis of the Kerrobert THAI (toe-to-heel air injection) operation in Saskatchewan. THAI is an air injection process where the injected oxygen reacts with the oil in the reservoir to create heat which mobilizes oil to the production well. The objective of this research is to fully evaluate the field production performance of the Kerrobert THAI project. Also, from data mining and analytics, the goal is to demonstrate the recovery mechanisms and the strengths and limitations of the process. In addition, Wei proposes improved operational strategies for ongoing operations and future project development. Another component of the research is to understand how in situ hydrogen is generated in the process.



Results

From simple observation of field data, it is demonstrated that data clusters (clumps) exist between toe temperature versus air injection and liquid production. Wei used clustering analysis to understand the production performance, and the result revealed clear data partitions between the low temperature and high temperature regions (low temperature oxidation reaction versus high temperature oxidation reaction). In the high temperature regime (more than 300 C), data is further separated by air injection criteria where higher air injection results in lower liquid production. It shows that there is competition between heat generation via oxidation reactions versus system cooling from excess air injections. The clustering analysis also identified liquid production is highest within the steam flashing zone in the mobilized oil region, and alternating injection-production recovery strategy may improve production performance.

Final remarks

- Clustering analysis provides new insights on how operating parameters contribute to production.
- Air injection rate is constrained for production maximization due to the balance between heat generation and cooling the combustion system by excess air supply.
- Cyclic injection-production strategy may improve process performance.

MEXICO RESEARCH COLLABORATION

The University of Calgary's partnership with Mexico will draw upon the university's world-leading expertise to solve complex challenges in technology, governance and regulation. The university recognizes the support through the Sectoral Fund provided by CONACYT-Secretaría de Energía-Hidrocarburos through the creation and incorporation of four knowledge networks. This partnership will tackle the specific challenges facing Mexico's hydrocarbon sector: scientific and technological research in the area of energy, development and deployment of technologies, training and capacity development in energy policy, regulation, business units and governance. Research projects such as these stand to advance both countries' efforts in reducing greenhouse gas emissions and increasing energy security.

KNOWLEDGE NETWORK 1

SOLUTIONS FOR HEAVY & EXTRA-HEAVY OILS

Ron Hugo, Roberto Aguilera, Pedro Pereira-Almao, Nashaat Nassar

- Tackle challenges and seize opportunities in extraction, transportation and processing of heavy and extra-heavy crude oils throughout the value chain of heavy crude oils in Mexico.
- Ensure that the policy and regulatory frameworks consider best practices to achieve a climate of competitive investment while also safeguarding environmental responsibility and safety in the extraction, transportation and processing of heavy crude oils.

KNOWLEDGE NETWORK 2

SOLUTIONS FOR MATURE OIL FIELDS AND UNCONVENTIONAL FIELDS

Hossein Hejazi, Sudarshan (Raj) Mehta, Jerry Jensen, Thomas Oldenburg, Per K. Pedersen, Robert (Gordon) Moore, Kimberly Johnston

- Tackle challenges and seize opportunities in extraction and processing in mature oil fields in Mexico's energy sector.
- Tackle challenges and seize opportunities in extraction and processing in unconventional oil fields in Mexico's energy sector.
- Study the geology of mature oil fields and unconventional oil fields.
- Ensure that the policy and regulatory framework consider best practices to achieve a climate of competitive investment, while also safeguarding environmental responsibility and safety in the extraction of resources from mature oil fields and unconventional deposits.

KNOWLEDGE NETWORK: SOLUTIONS FOR HEAVY AND EXTRA-HEAVY OIL

Ron Hugo, Roberto Aguilera, Pedro Pereira-Almao, Nashaat Nassar

Projects

Determination of rock compressibility in unconsolidated sands and fractured carbonates in heavy and extra-heavy oils reservoirs: The University of Calgary is contributing jointly with its Mexican partners to increase the recovery rate in Mexico. Dr. Roberto Aguilera's team is generating a methodology for accurately calculating rock compressibility in heavy and extra-heavy oil deposits, mainly in unconsolidated sand formations and naturally fractured carbonate reservoirs. This has the potential to increase the recovery rate by 10 per cent. The positioning of the different elements that make up a reservoir, such as faults, wedges, lithology changes, discordances and contacts of fluids, will play an important role in the dynamic characterization of the reservoirs.

Integrated thermal enhanced oil recovery — in reservoir catalytic upgrading: This research project, conducted by Dr. Pedro Pereira-Almao's team, employs and tests nano-catalytic technologies that may enable the more efficient recovery of oil from Mexican heavy oil reservoirs. Pedro's team will adjust, optimize and further develop for off-shore application, the in situ upgrading invented and experimentally developed at the University of Calgary since 2011. This enhanced oil recovery process will consume only a small fraction of the energy content of the produced oil, utilize energy from the least desirable fraction of the bitumen (i.e., the very heavy ends that are laden with sulphur and toxic metals), release a minimum amount of greenhouse gases into the atmosphere and produce no wastewater or solid waste materials, consume very little fresh water and produce oil that is of higher quality than the in situ resource, not requiring dilution to be pipelined.

Aqua processing for offshore and field upgrading of extra-heavy oils research: This research attempts to apply catalytic aqua processing technology (AQP), recently invented at the University of Calgary, to Mexican heavy oil fields. AQP improves the quality of heavy and extra-heavy oils at the surface, either at the well level or at the discharge or battery, thanks to the reduction of viscosity it achieves. AQP consists of carrying out on-site hydro processing with steam using a catalyst in a simple low footprint facility. Dr. Pedro Pereira-Almao's team is working on this project that will be applicable at surface installations, both on land and on marine platforms, allowing heavy and extra-heavy oil to be easy to transport.

Analysis of the effect of a bio-drag reducer on the enhancement of the flow of heavy and extra-heavy crude oils in vertical pipes: This project will develop, evaluate and apply in the field a bio-drag reducer (made by biodiesel) to improve the flow in vertical wells, deviated and surface facilities. This technology will be applied to Mexican heavy and extra-heavy oils typically produced in the fields of the Northeast Marine Region. The research conducted by Dr. Ron Hugo's team will characterize and assess the compatibility of the bio-reducer with oils of interest. Pilot tests will be performed to fully assess the effects of the bio-reducer. An injection method will be designed and analyzed using a variety of flow sensing systems. An injection system design will be developed, and an operational strategy for application of the bio-reducer in production fields established.

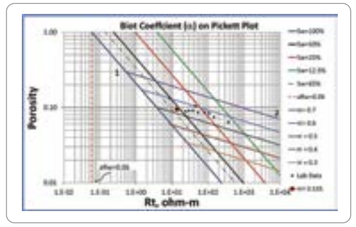
Development of an oxy-cracking process scheme for demineralizing (metals removal) and converting petroleum coke into commodity chemicals: In Mexico, petcoke is used as an alternative to coal given its higher calorific value and lower ash content. However, due to its content of minerals like vanadium, nickel and iron, and heteroatoms like oxygen, nitrogen and sulfur, petcoke burning produces Sulphur oxides (Sox), nitrogen oxides (NOx), and particulates that are considered major pollutants to the environment. Dr. Nashaat Nassar's team is working on demineralizing and removing the heteroatoms from the petcoke before burning it. This technique minimizes the path to CO_2, is cost-effective and favors the production of humic acid analogs, a major organic constituent of soil.

Determination of rock compressibility in unconsolidated sands and fractured carbonates in heavy and extra-heavy oils reservoirs

Bukola Korede Olusola
PhD student

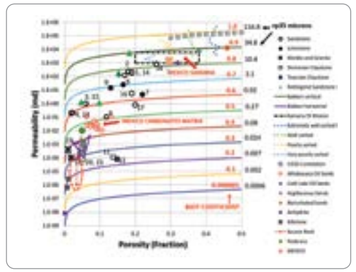
Introduction

Dr. Bukola Olusola, PhD, aimed to integrate Biot coefficient, porosity, water saturation, permeability and pore throat aperture. He was successful in his efforts and managed to link petrophysics and a correlation developed by his research team for estimating Biot coefficient. Bukola performed the integration of petrophysics and Biot coefficient using a Pickett plot. This was the first time that petrophysics and geomechanics were integrated in a single graph.



Results

Bukola worked with drill cuttings of Mexican carbonates. His work in the laboratory at the University of Calgary permitted determination of porosities, permeabilities and extensions for estimating geomechanical parameters such as Biot coefficient, Young's modulus and Poisson's ratio. Due to his research, Biot coefficient, water saturation, porosity, permeability, capillary pressure and pore throat apertures for a given reservoir interval were observed for the first time in the same graph.



Final remarks

- This research incorporated for the first time the petrophysical analysis and Biot poroelastic coefficient.
- The proposed Pickett plots permits quick, simultaneous pattern-recognition estimation of different parameters of interest for a given interval including, for example, water saturation, porosity, permeability, pore throat aperture and Biot coefficient.
- There is a general tendency for Biot coefficient to decrease as water saturation increases.
- There is a general tendency for Biot coefficient to increase as porosity, permeability, process speed and pore throat aperture increase.
- The integration of petrophysical parameters and Biot coefficient in a single Pickett plot provides a new valuable tool to assist in the solution of petroleum engineering problems such as hydraulic fracturing and estimation of in situ closure stress on proppant.

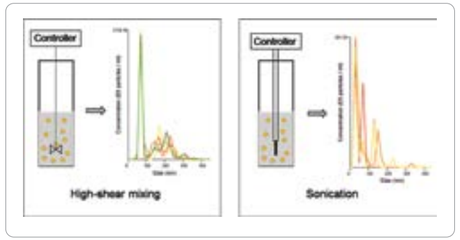
Integrated thermal enhanced oil recovery — in reservoir catalytic upgrading

Hybrid steam-assisted in situ upgrading technology of heavy oil and bitumen

Milad Ahmadi Khoshooei
PhD student

Introduction

Milad Ahmadi Khoshooei aims to partially replace hydrogen with steam to reduce both the cost and environmental footprint of in situ upgrading technology (ISUT). This method employs nanocatalysts to upgrade the oil downhole. Hydrogen is required to carry out hydroprocessing reactions to upgrade the injected vacuum residue. He is investigating the effects of steam on different catalysts in terms of activity and selectivity. His main aim is to find a suitable catalyst, with water splitting capability, to abstract hydrogen from water molecules to successfully replace hydrogen. The selected catalyst should be stable and active at reservoir conditions.



Results

Milad has investigated the application of ultrasound for preparing nanocatalysts for ISUT. Using this method, more active catalysts were synthesized, probably owing to the smaller size of the produced catalyst. The smaller size can be attributed to the better admixing effect, owing to the sufficiently high energy density generated via ultrasonication, as compared to conventional high-shear mixing.

He has also found that the conventional nickel-molybdenum (Ni-Mo) catalyst used in ISUT technology is impacted by the presence of steam. The conversion of vacuum residue has increased while the hydrogenation capabilities have supressed. In particular, the microcarbon content, desulphurization and asphaltene reduction was impacted under the hybrid environment of hydrogen and steam, with the molar ratio of one to one. The hydrogenation suppression was also explicitly monitored by the hydrogenation of phenanthrene, where the hydrogenation dropped significantly once steam was also introduced in the system along with hydrogen.

Final remarks

- The Ni-Mo nanocatalyst prepared using ultrasound results in higher activity of hydrogenation and hydrodesulphurization in the ISUT method.
- A water splitting catalyst is needed to successfully abstract hydrogen from water to partially replace hydrogen. This phase of the project will be further researched by Milad to effectively reduce the costs and environmental footprints of the ISUT method.

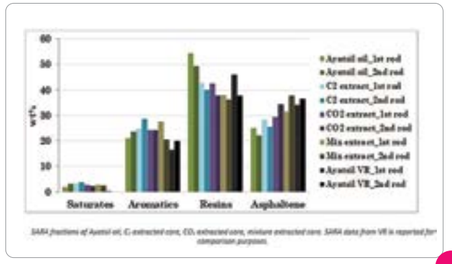
Integrated thermal enhanced oil recovery — in reservoir catalytic upgrading

Experimental and numerical investigation of cyclic solvent injection in heavy oil carbonate resources

Yasaman Assef
PhD student

Introduction

Due to increasing energy demand and fast depletion of conventional oil resources, a strong interest exists in unconventional oil production, namely, extra-heavy oil from naturally fractured carbonates. The heterogeneous nature of these types of reservoirs, along with their low matrix permeability and porosity, have been known as major constraints for implementing the conventional gas flooding technique. Gas breakthrough along the fractures does not allow the injected fluid to effectively contact the oil in the matrix. Cyclic gas injection (CGI) has been recognized as an effective recovery technique in which the injection and production occurs in a single well.



SARA fractions of Ayatsil oil, C2 extracted core, CO2 extracted core, mixture extracted core. SARA data from VR is reported for comparison purposes.

Results

Yasaman Assef has conducted a series of experiments to determine the efficiency of CGI in extra-heavy oil carbonates under high pressure and high temperature. She considered carbon dioxide (CO_2), ethane, propane and a mixture of solvents (0.5CO_2 and 0.5C_2) and (0.5CO_2 and 0.4C_2 and 0.1C_3) with different propane concentrations. According to her simulation results, ethane acts as a stronger solvent than CO_2 in extracting IC_5-C_{12}, while performing similar to CO_2 in producing heavier components of C_{13}-C_20, C_{21}-C_{45} and C_{45}-C_{45}+. Most of the extraction occurs during the first and second cycles, which is consistent with the rate of pressure decay records. Compared to CO_2, ethane leads to more efficient gas dissolution, oil viscosity reduction and a higher degree of oil swelling. Addition of C_3 to the mixture increases the solubility of the solvent, mass transfer and the degree of swelling effect.

Final remarks

- Negligible oil production in later cycles is due to the lack of effective solution-gas drive.
- The foamy behaviour was observed during the very early phase of the first cycles while it was hardly seen in later cycles.
- Saturates, Asphaltenes, Resins and Aromatics (SARA) analysis confirmed asphaltenes precipitation during CGI at high pressure, which may be accelerated by adding a deasphalting agent such as propane.
- Distillation curves illustrate loss of light hydrocarbon components during production cycles when the samples are flashed at atmospheric pressure.
- As diffusion coefficient is a determinant factor as a function of required time to achieve optimum recovery, the molecular diffusivity data obtained from the study can be deployed for properly designing a potential solvent-based enhanced oil recovery process in the Ayatsil reservoir.

Integrated thermal enhanced oil recovery — in reservoir catalytic upgrading

Lante Carbognani
Research Associate

Introduction

Lante Carbognani, worked on creating a catalytic zone around the injector well by dispersing nanometric nickel-molybdenum (Ni-Mo) sulphided particles in vacuum residue (VR) and flowing them into a sand-packed mimic of the Samaria reservoir. He evaluated dispersion under high shear stress and ultrasonic energy. He then explored patented in situ upgrading technology (ISUT) at around 320-350 C with small contents of hydrogen. Lante studied hydrogenation under varying amounts of reservoir water, showing how important this parameter is for achieving different hydrogenation and/or cracking conversion levels. A spiked molecular marker (phenanthrene) was used as proxy for understanding the progress of aromatics hydrogenation.

Results

Lante collaborated on the creation of a soon-to-be-published article discussing how ultrasonic energy was found to be better for achieving smaller nanoparticle sizes. Figure 1 shows that the presence of water decreased ISUT conversion of Samaria VR (less cracking) and decreased phenanthrene reactivity to hydrogenation. Desulphurization was found to depend on the presence of water, decreasing when water increases. Rationalization of the preceding findings indicates that Ni-Mo-sulphided catalytic species are interconvertible to oxisulphides.

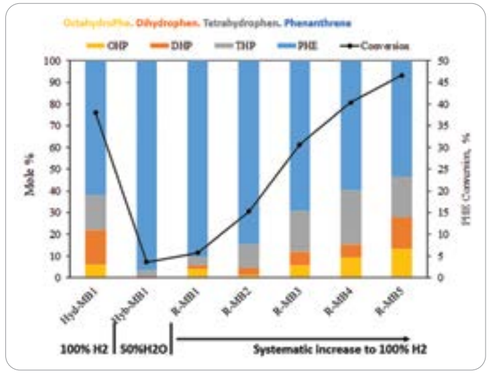


Figure 1

Final remarks

- Ultrasonics provide better catalyst dispersion than high-shear mixers.
- Successful ISUT processing conditions for Samaria VR/Samaria oil is demonstrated.
- Water affects catalysts transformation into oxisulphides providing different crackability and product selectivity.
- An aromatic molecular marker (phenanthrene) is an effective proxy for hydrogenation reaction monitoring.

Integrated thermal enhanced oil recovery — in reservoir catalytic upgrading

Study on Mo nanoparticle deposition modeling for application in in situ upgrading technology

Antonio Garcia Vila
PhD student

Introduction

Antonio Garcia Vila is currently developing a nanoparticle deposition model to predict how nanoparticles diffuse and adsorb into sandstone reservoirs. The study is focused on the application of in situ upgrading technology, developed at the University of Calgary by Prof. Pedro Pereira-Almao's group, to a Mexican sandstone reservoir. The main goal is counting nanoparticle distribution with a model capable of describing the formation of an underground reactor to carry out upgrading reactions. The resulting upgraded oil will offer advantages like permanent viscosity reduction and an increase in valuable oil fraction compared to the original oil in the reservoir.

Results

Antonio is developing an analytical procedure based on X-ray fluorescence to determine molybdenum, nickel and vanadium concentrations in heavy crudes, heavy residual cuts, sandstones and carbonates. This analytical procedure will lead to accurate measurements on the distribution of nanoparticles over physical models of reservoirs.

As evidence from previous studies shows, these particles adsorb irreversibly in the reservoir matrix. Now, the challenge is to describe the mechanisms that follow this adsorption. The ongoing research has led to the commissioning of a new pilot unit to recreate the conditions of Mexican Samaria reservoir and study the adsorption of nanoparticles at those conditions. In this sense, the technology developed by Antonio and Prof. Pereira-Almao's research group at the University of Calgary has a direct application to a technology gap in Mexico.

Final remarks

- The understanding of nanoparticle adsorption will help to comprehend how upgrading reactions take place.
- The distribution of these nanoparticles will give the research team information about the underground reactor formation and performance to carry out the upgrading reactions.
- The analytical procedure continues to be refined to obtain precise data to be used to build the nanoparticle deposition model.
- A pilot unit will be constructed to recreate the conditions of the Samaria sandstone reservoir, proving that the technology can be applied to actual non-conventional oil production projects in Mexico.

Integrated thermal enhanced oil recovery — in reservoir catalytic upgrading

In situ upgrading of Mexican heavy oils using nano-catalytic hydroprocessing

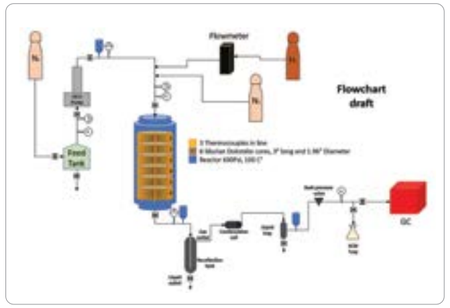
Javier Marti
MSc student

Introduction

Javier Marti's focus is to utilize huff and puff technology experiments to demonstrate the capabilities of the nano-catalytic hydroprocessing technology and its huge advantages to upgrade and recover oil in naturally-fractured carbonates.

The huff and puff application consists of injecting oil containing nanocatalysts and hydrogen into the reservoir at a temperature between 320 C and 340 C, leaving a soaking period of no more than two days. The oil is injected through the same injector well in which the oil is produced, and a portion of the oil produced is reinjected to restart the cycle. This process is repeated until the oil in place is close to depletion.

To simulate the process, Javier is building a lab pilot plant to run experiments at the reservoir conditions in minimum two dimensions. He will also perform tests with different operational conditions to highlight the advantages of this technology. Finally, he will characterize the products obtained during the different experiments through a battery of characterization techniques available with the Catalysis and Adsorption for Energy and Fuels Research Group at the University of Calgary.



Results

Javier continues to work on the completion of the pilot plant unit. He believes that the unit will allow him to run experiments that will confirm the efficiencies of the process, its huge operational advantages, its high level of upgrading and its more than competitive oil recovery potential as evidenced by pioneer experiments by other colleagues and numerical simulations of carbonate reservoirs already performed.

Final remarks

- The unit construction will be fast because all the materials and equipment needed are in stock.
- Due to previous experiments, a wide range of knowledge on the construction of this setup is available to Javier.
- The nanocatalyst technology has been tested several times and proved its in situ upgrading capabilities and attractiveness for heavy oil production.
- The relative simplicity of the process is appealing and interesting from an operational perspective.

Integrated thermal enhanced oil recovery — in reservoir catalytic upgrading

Chemical functionalities reactivity during partial steam reforming of hydrocarbons

Diego Moreno
PhD student

Introduction

Diego Moreno's goal is to explain the behaviour of nickel-cerium catalysts during naphthenic acid removal and low catalytic steam reformation, with the aim of using this information for optimizing hydrogen production.

Results

Diego has delivered one report to his industrial sponsor that shows promising results in hydrogen production from biofuels. He is in the process of publishing two academic papers with most recent results.

Final remarks

- Diego demonstrated that catalytic naphthenic acid removal carried at lower pressure has different behaviour than what is expected at higher pressure.
- He demonstrated that when low catalytic steam cracking of light gases blend, gases heavier than methane (e.g., ethane and propane) promote a methanation reaction.
- Optimization of hydrogen production has been reached.

MEXICO RESEARCH COLLABORATION

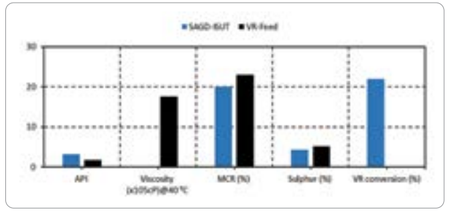
Integrated thermal enhanced oil recovery — in reservoir catalytic upgrading

Experimental and numerical modelling of hybrid steam and in situ upgrading process for immobile oil

Violeta Wills
PhD student

Introduction

This project presents an integrated concept for recovering and upgrading bitumen using in situ upgrading technology (ISUT), which replaces a significant amount of the steam injected by steam-assisted gravity drainage (SAGD) with a hot catalytic mixture that includes the heaviest fraction of the bitumen itself and hydrogen. Therefore, the hybrid SAGD-ISUT is an alternative option of upgrading the oil in the reservoir to produce a synthetic crude oil that meets the pipeline requirements by addressing the costs, deficiencies of diluents and environmental emissions.



Results

As part of this project, a new experimental setup was designed and validated. The relatively small and simple configuration of this elemental model facilitated the operating procedures of packing, saturation and mass balances collection which led to reproducible results that guaranteed an adequate representation of the steam injection processes simulated. Additional advantages perceived for this system are the potential reduction of time and costs for assembling and maintaining the model. Moreover, the versatility of the unit would permit the evaluation of thermal and non-thermal recovery methods such as huff and puff and waterflooding with a different well scheme.

The simplicity of this experimental model also brought the possibility of efficiently creating numerical simulation replicas that complement the laboratory experimentation.

Results obtained from the newly designed unit and numerical simulation confirmed the superior performance of the reactive hybrid SAGD-ISUT, regarding 40 per cent usage of steam with close to 30 per cent enhancement of oil in place recovery.

Final remarks

- Almost identical matching trends for the experimental steam injection in the designed unit and for SAGD reservoir simulations were found.
- The catalytic SAGD-ISUT concept of simultaneous recovery-upgrading was demonstrated in a new experimental unit.
- The quality of the products obtained via SAGD-ISUT provides evidence that the catalyst promoted hydroprocessing reactions inside the porous media.
- Numerical simulation showed the potential of hybrid SAGD-ISUT to enhance the oil recovery by 30 per cent compared to the conventional steam injection method while reducing the cumulative steam-oil ratio by about 22 per cent and greenhouse gas emissions by 15 per cent.

Aqua processing for offshore and field upgrading of extra-heavy oils research

Lante Carbognani
Research Associate

Introduction

A single-pass catalytic processing approach, i.e., no ancillary techniques required (example: distillation), was demonstrated at bench-scale. Patented solid catalysts containing active metallic species including, nickel, molybdenum, cerium, allow upgrades to heavy oil with noticeable viscosity reductions (more than 98 per cent) and high (80-100 per cent) acidity reduction. Water is the participating reagent that catalytically generates hydrogen mostly under cerium action, then hydrogen is transferred under the effects of the other metallic species. This process is called aquaprocessing. Lante Carbognani is involved in the characterization of feedstock and upgraded products, which provides the data necessary for ascertaining the success and the understanding of performed tests with oil from the Samaria reservoir.

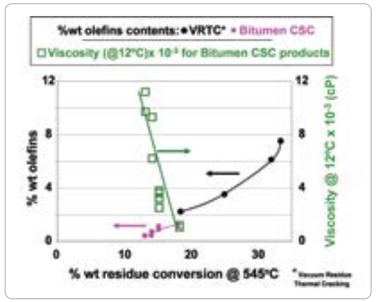


Figure 1

Results

Characterization results showed how catalytic hydrogen production followed by hydrogenation of oil components enhanced product-quality parameters. Figure 1 highlights how catalytic steam cracking (CSC) applied to whole heavy oil precludes the production of olefins much better compared to thermal cracking. Low viscosity levels attained for bitumen CSC are also presented in Figure 1.

Lante has worked with Jesus Fuenmayor, whose recent MSc thesis results showed how alumina-based CSC catalysts with wider and controlled porosity provided optimized results for Samaria oil.

Final remarks

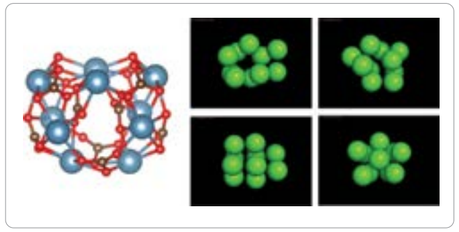
- CSC is a very attractive upgrading schematic because a very simple process is involved.
- CSC has been found to provide noticeable upgrading for bitumen/heavy oils.
- Water-based CSC upgrading is very attractive for partial heavy oils upgrading (low-cost option).
- Wider pore alumina-based catalysts are better for heavy samples (like Samaria oil).
- Samaria oil is less reactive than Alberta's tested bitumen (this Mexican oil is more polar and more hydrogen deficient).

Aqua processing for offshore and field upgrading of extra-heavy oils research

Jiri Hostas
Postdoctoral Fellow

Introduction

Due to its high viscosity, unconventional oil cannot be recovered using conventional drilling. One way to tackle this challenge is to use a catalytic system for upgrading extra-heavy oil, which lowers the feedstock viscosity. In the past, the studies of catalytic processes have been greatly assisted by efficient and accurate electronic structure methodologies, most notably density functional theory (DFT). Dr. Jiri Hostas, PhD, is interested in combining DFT and machine learning methods to study molybdenum sulphide (MoS_2), a hydrogenation and coke-prevention catalyst.



Results

Jiri has performed the exploratory calculations of interface between MoS_2 nanoparticles (NPs), models of rock and asphaltenes. These initial calculations pointed him towards a systematic study of calcium carbonate ($CaCO_3$) and molybdenum disulfide (MoS_2) flexibility using DFT and Born-Oppenheimer molecular dynamic (BO-MD) simulations. These simulations provide not only information about the material flexibility for material chemists but also help in providing an enormous amount of data needed for the development of novel machine learning techniques. Jiri developed a deep neural network predictive model specific to MoS_2 which has been very successful in emulating $(MoS_2)_{16}$ DFT energies. This work has potential to vastly increase the applicability range of the methodology, especially when used within an adaptive BO-MD approach.

Final remarks

- Jiri concludes that the asphaltene sulphur atoms play a key role in the formation of a direct bond with the active Mo-edges of the MoS_2 catalyst.
- He found new local minima for (MoS_2), with eight and 16 units; NPs which will be used as starting points for free energy calculations in the future.
- He is developing deep a neural network predictive model as an alternative approach for studies of larger MoS_2 nanoparticles.

Jiri acknowledges NSERC Discovery Grants for support of this work and Compute Canada and WestGrid for the provision of computational resources

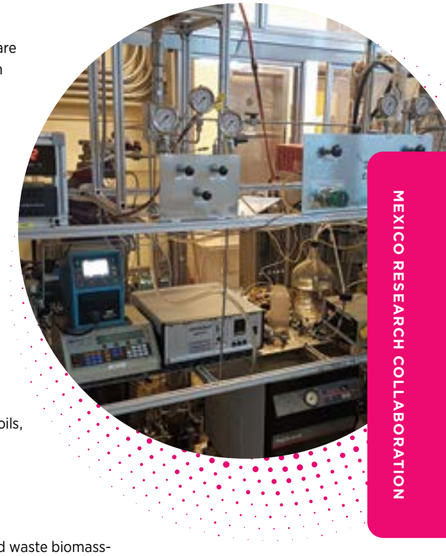
Aqua processing for offshore and field upgrading of extra-heavy oils research

Ultrasound-assisted oxidative desulfurization of heavy fuel oil and waste biomass derived fuels

Florian Isufaj
PhD student

Introduction

Florian Isufaj is participating in the development of a sulphur oxidative-process incorporation before aquaprocessing to enhance the performance of the field upgrading method. Two of the feedstocks that are being targeted are high-sulphur oils (where sulphur is to be reduced to 0.5 weight per cent). His research goal is to study all the process parameters that can alter and optimize the aquaprocessing technique, in terms of achieving the target sulphur content while lowering the reactants and energy consumption.



Results

Florian has participated in the design and construction of two pilot plant units that are operated in continuous mode following the ultrasound-assisted oxidative desulphurization (UAOD) process. He has performed experiments to identify the variables that affect the process, such as ultrasound processor-related variables, residence time, temperature, etc. One of the successful results so far has been the reduction of sulphur in the target oil, from 1.4 weight per cent to 0.7 weight per cent sulphur content in the final product. It is very close to the allowed 0.5 weight per cent that is required today by the shipping industry.

Final remarks

- After being successful in demonstrating that this technology can work in the desulfurization of heavy oils, the next step is the optimization of the process variables.
- The targets are:
  - Maximizing the sulphur removal while maintaining or even upgrading the oil quality.
  - Lowering the process cost.
- Florian will be continuing to improve this technology and adapt it for treating lighter hydrocarbons and waste biomass-derived fuels as well.

MEXICO RESEARCH COLLABORATION

Aqua processing for offshore and field upgrading of extra-heavy oils research

Lilia Prieto Araujo
MSc student

Introduction

Lilia Prieto Araujo aims to contribute to the development of aquaprocessing as a well-established partial-upgrading technology for its field test and future commercial application in Mexico and beyond. To achieve this, Lilia intends to analyze the kinetics of Samaria oil to optimize both operational parameters and catalyst design. Additionally, she will study the aquaprocessing application path when coupled to another upgrading technology, such as hydrotreating. Finally, she will study the application of aquaprocessing to different oil cuts and heavy oil feedstocks with different catalysts designed by the Catalysis and Adsorption for Energy and Fuels Research Group at the University of Calgary.

Results

Lilia expects to contribute to a better understanding of the partial-upgrading process using aquaprocessing technology, so it can be fully developed for commercial applications. This is a promising technology for the oil industry and, in particular, for Mexico and Canada because it can achieve the minimum specifications for pipeline transportation with a substantial decrease in prices compared to current upgrading processes. This will decrease the costs of oil production and will increase the competitiveness of oil as an energy source, thus favouring the economy of oil producing countries.

Final remarks

- Multiple operational conditions need to be tested using an aquaprocessing pilot plant to achieve the optimal parameters for a given crude oil and catalyst.
- Coupling aquaprocessing with other partial-upgrading technologies may significantly enhance the properties of different feedstocks, making it important to study.

Aqua processing for offshore and field upgrading of extra-heavy oils research

Reactor design and optimisation for aquaprocessing and in situ technology

Alireza Zarrabian
MSc student

Introduction

Alireza Zarrabian aims to develop a practical reactor design to best suit the requirements of the Samaria reservoir for in situ and aquaprocessing applications.

Results

Dr. Pedro Pereira-Almao and his team have proven a novel and very efficient methodology to dilute and extract Samaria oil using oil residue. Alireza, using his background knowledge in mechanical engineering, joined the research team and he is trying to optimize the reactor design to best fit scaled-up application of the technology in the field.

Final remarks

- Alireza will verify the reactor's design from the fluid mechanics and heat transfer perspectives.
- He will build the reactor and use it in pilot scale to evaluate its mechanical integrity.
- He will design modifications for scale-up in the field.

Analysis of the effect of a bio-drag reducer on the enhancement of the flow of heavy and extra-heavy crude oils in vertical pipes

Haydee Coronado Diaz
Postdoctoral Fellow

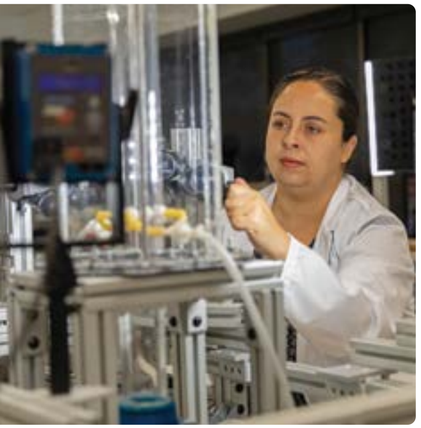


Figure 1

Introduction

A bio-drag reducer has been developed at the National Autonomous University of Mexico to enhance the production of heavy and extra-heavy oils in Mexican wellbores. Dr. Haydee Coronado Diaz, PhD, aims to design a reliable injection system for the bio-drag reducer. She is designing and building a non-invasive vertical multiphase flow facility and develop a simulation model. She uses glycerine and glycerine-water mixtures to simulate the flow of heavy oil and the bio-drag reducers in a transparent section of the flow facility, and applies an optical tomography system formed by a set of three high-speed sensors to characterize the multiphase flow patterns with different injection arrangements.

Results

Haydee, along with the rest of the team, has developed an image-processing technique to considerably reduce the error in volumetric reconstruction of vertical multiphase flow patterns with high-speed sensors. Figure 1 shows the vertical flow facility built and the incorporated injection system. She has analyzed the injection of varying viscosity fluids into glycerine using up to four concentric nozzles. She is currently developing a numerical simulation that will be verified using experimental data.

A non-intrusive system to measure volumetric concentration, enabling tracking of glycerine-water mixtures into the glycerine, is also under development.

Final remarks

- A comprehensive image characterization has demonstrated the feasibility of the optical tomography system for different multiphase flow regimes.
- The design of an optimum injection system is ongoing and will allow for the improvement of the use of the bio-drag reducers in field applications.

Analysis of the effect of a bio-drag reducer on the enhancement of the flow of heavy and extra-heavy crude oils in vertical pipes

Experimental study of highly-viscous vertical pipe flow using an optical tomography system

Miriam Solis Meza
MSc student

Introduction

Miriam Solis Meza is investigating the fluid dynamics present in offshore oil production risers by performing experiments on the vertical multiphase flow of a highly viscous fluid, a lower-viscosity drag-reducing agent and air bubbles. She is examining the behaviour of air bubbles as they ascend vertically in both high- and low-viscosity zones. The goal of her research is to both track and quantify bubble geometry using a non-intrusive optical measurement technique. This information will be used to improve the application of drag-reducing agents to the production of extra-heavy oil.

Results

Miriam has designed and assembled an experimental apparatus using an optical tomography system that tracks the rise of bubbles in a quiescent fluid with both high- and low-viscosity regions. She developed a digital image processing algorithm that reduced optical artifacts that contributed to measurement errors. The algorithm uses a morphological approach to process data for both moderate- and strong-shape deformations. This improves both bubble tracking and volumetric quantification as bubbles rise through a vertical pipe. An improvement in the tracking and volumetric quantification of bubbles rising through columns with varying viscosity helps to better understand the mixing that occurs when drag-reducing agents are injected into vertical production risers during production of ultra-heavy oil.

Final remarks

- The developed algorithm reduces the impact of strong-light reflections on the edge detection process.
- Edge detection procedures have been investigated statistically to improve system accuracy.
- The developed algorithm can estimate bubble volume with errors ranging from 4.7 per cent for the uniform viscosity column to 4.9 per cent for the stratified viscosity column.

Development of an oxy-cracking process scheme for demineralizing (metals removal) and converting petroleum coke into commodity chemicals

Azfar Hassan
Research Associate

Introduction

Dr. Azfar Hassan, PhD, is researching thermal and chemical reactivity of oxy-cracked products using Thermogravimetry-differential thermal analysis (TG-DTA), Fourier-transform infrared spectrometry (FTIR) and other spectroscopic techniques. The focus is on finding new routes to valuable products from heavy-oil waste hydrocarbons using oxy-cracking technology. At present, his work is geared towards the formation of carbon fibres with high tensile strength.

Results

Azfar evaluated the thermal stability and the reactivity of oxy-cracked products under oxidative and non-oxidative conditions. His results showed that the oxidized products are thermally more reactive than the precursor material and have the potential to be used in forming valuable products such as carbon fibres. The TG-DTA data shows that a good portion of water-soluble product obtained after oxy-cracking of asphaltenes has similar trends of reactivity to commercially-available humic acid.

Final remarks

- The oxy-cracking technology leads to metal-rejection vanadium and nickel, and the formation of more oxidized products.
- Because of heavy-metal rejection, the oxy-cracked material has the potential to be used in formation of valuable products such as carbon fibres.
- This technology leads to the formation of a variety of oxidized products with a potential to be used in the fabrication of many commercial products.

Development of an oxy-cracking process scheme for demineralizing (metals removal) and converting petroleum coke into commodity chemicals

Abdallah Manasrah
Postdoctoral Fellow

Introduction

Dr. Abdallah Manasrah, PhD, is focused on the application of oxy-cracking technology for converting the residual feedstocks like petroleum coke (petcoke) and mine-reject asphaltenes into valuable products such as humic acids, clean fuel, carbon nanomaterials and carbon fibres. This alternative and cost-effective technique can also be used for recovering valuable metals like vanadium and nickel. This novel technique is a combination of oxidation and cracking reactions occurring simultaneously in an aqueous alkaline media at moderate temperatures (approx. 170 C) and pressures (300-500 pounds per square inch) with relatively low proportions of water.

Results

Abdallah evaluated the effects of oxy-cracking reaction conditions on petcoke, such as temperature, oxygen pressure, reaction time, particle size and mixing rate to optimize the conversion and selectivity of oxy-cracked products. The results show that the temperature and the residence time are the two major important parameters that affect the reaction yield and cause environmental impact. The characterization results of oxy-cracked products, using Fourier-transform infrared spectrometry (FTIR), nuclear magnetic resonance (NMR), thermogravimetric analysis (TGA), and X-ray diffraction (XRD) let Abdallah conclude that the main oxy-cracking product is humic acid, which can be used for many applications including as an organic fertilizer. He successfully managed to describe the reaction kinetics mechanism of the oxy-cracking process based on the hydroxyl radical using the triangular lumped kinetics model where the residual feedstocks are simultaneously oxy-cracked to produce oxygenated hydrocarbons soluble in water. Such innovative technology might have a significant impact on the energy and environment sectors, as it will not only reduce the environmental impact of the oil industry, but it will also improve the economy and sustainability of oil operations.

Final remarks

- The oxy-cracking technology has multiple product pathways, each addressing a unique technical and business opportunity.
- Oxy-cracking is a back-end technology for several value-added non-combustion chemical products such as humic acids, lighter hydrocarbons, carbon nanomaterials, graphene, carbon fibres and composites, and recovering valuable metals like vanadium and nickel.
- The key benefit of this technology is not only the high efficiency, conversion and selectivity for desired products but also zero direct CO_2 emissions.
- This technology could also be applied to demineralization and desulphurization of residue streams.

KNOWLEDGE NETWORK: SOLUTIONS FOR MATURE OIL FIELDS AND UNCONVENTIONAL FIELDS

Hossein Hejazi, Sudarshan (Raj) Mehta, Jerry Jensen, Thomas Oldenburg, Per K. Pedersen, Robert (Gordon) Moore, Kimberly Johnston

Projects

Enhanced oil recovery from naturally fractured and sandstone reservoirs using air injection technology: Many Mexican naturally fractured reservoirs (NFRs) have been contaminated by water from nearby aquifers, by gas from a nearby gas cap, and/ or by injected gases such as the nitrogen gas that is often injected in oil reservoirs to help force out oil. Dr. Sudarshan Mehta, PhD, aims to understand the key mechanism for air injection for NFRs as well as sandstone reservoirs, and specifically, to learn how to initiate and control the process under conditions that are unique for each of the reservoirs.

Optimizing oil extraction from mature fields through the analysis of interwell connectivity: Many Mexican reservoirs have thick (heavy) oil and poor rates of recovery using existing methods for extracting that oil. In the national and international hydrocarbon sector, there is no technological platform or methodology that integrates the modelling of connectivity between wells with the reevaluation of the static model (conditioning of geological-petrophysical models). To develop a methodology of this type would allow the conditioning of static ad hoc models to the dynamic behavior of mature fields, which would allow optimization of the production and development of these mature fields. The goal of this project is to improve the extraction of oil from mature reservoirs through analyzing how the flow of oil from producer wells changes due to pumping water into the reservoir through nearby injector wells.

Integrated fluid characterization and reservoir compartmentalization identification using geochemical techniques: The final viscosity of oil depends on numerous factors, and such factors can lead to oils with very different fluid properties existing within the same reservoir. Dr. Thomas Oldenburg, PhD, and his research group work on identifying these variations, vertically and laterally, in selected Mexican reservoirs by analyzing fresh oils and cuttings using advanced geochemical techniques such as Fourier-transform ion cyclotron resonance mass spectrometry (FTICRMS). In combination with geological information and reservoir engineering, a comprehensive methodology will be developed to define a more robust compartmentalization and fluid distribution reservoir model to support the design and implementation of new exploitation strategies in mature oil fields.

Advanced characterization and innovative solutions for the recovery of the heavy oil in mature fields: In the Tabasco state of Mexico, subsurface petroleum reservoirs contain large, untapped volumes of heavy oil which require special treatment before it can be produced. Production engineers must force steam under high pressure into the reservoir to break down the heavy oil into lighter molecules so it can be pumped as liquid oil to the surface. Dr. Per K. Pedersen, PhD, and his team are working on locating the best reservoir rocks around the town of Villahermosa, Tabasco, and understanding their distribution through descriptions of subsurface rock samples and evaluation of subsurface data. The research also involves transfer of knowledge to production personnel and engineers who are directly involved in the production of the Mexican reservoirs

Using nanofluids and micro-reservoirs to enhance oil recovery from mature fields in Mexico: In most oil fields, more than two-thirds of the oil remains locked in underground rocks even after flooding the reservoir by water. Dr. Hossein Hejazi, PhD, and his team are developing innovative EOR methodologies, based on the inclusion of interfacial materials in the form of nanoparticles and surfactant injected from the surface or produced in situ. They are developing a robust microfluidic platform, referred to as microreservoirs, for visualization of fluids' interfaces at the pore level. This will lead to a new generation of lower cost smart fluids that can yield in situ interfacial materials for oil recovery from mature oil fields in Mexico.

Optimizing oil extraction from mature fields through the analysis of interwell connectivity

Gabriela Morales German
PhD student

Introduction

Considering waterflooding in heavy oil reservoirs, Gabriela Morales German's objective is to estimate the connectivity between injector and producer wells at early production by implementing the capacitance-resistance model (CRM) approach. To fulfill this objective, she needs to modify the current connectivity estimation methodology so that the heavy oil characteristics are properly taken into account.

Additionally, she will optimize the CRM approach by using an analogy between the equations describing heat flow and fluid flow in porous media. This will benefit the analysis by offering interwell connectivity estimates by analyzing injection disturbance as heat emittance.

Results

Existing methodology to measure interwell connectivity using the CRM approach was designed to be applied in medium and light oil reservoirs, thus, its implementation in heavy oil reservoirs needs to be adapted so the contrasting fluid properties are considered. When analyzing interwell connectivities based on the CRM formulation, it is paramount to pay special attention to the mobility variations through time and to effective water injection.

Gabriela's work will study the connectivity of such fluctuations at early time and proposes to modify estimation methodology so that accurate interwell connectivity can be estimated using early time production data. The steps followed in her study will include generating production data based on a synthetic model and sensitivity analysis of the main fluid properties and production variables, identifying stabilized connectivity values for heavy oil reservoirs, and developing a corrected method for early stabilized connectivity estimation.

Final remarks

- Fluid viscosity affects stabilization of connectivity estimates. The more viscous the oil is, the later the stabilization time is reached.
- General linear correlations relating connectivity parameters and injection volumes and rates may be used to estimate early time connectivities in a homogeneous medium.
- Final results may offer information related to bypassed oil, conduits and flow barriers, and other behaviour related to immiscible displacement processes and oil production in heavy oil reservoirs.

Optimizing oil extraction from mature fields through the analysis of interwell connectivity

Natalia Quintero
MSc student

Introduction

Heavy oil represents a large portion of proven oil reserves in the world. Nevertheless, its limited mobility in porous media leads to poor recoveries (three per cent to 10 per cent). In Mexico, as much as 62 per cent of the proven oil reserves and 54 per cent of the daily production correspond to heavy oil reservoirs. Natalia Quintero is implementing an alternate reservoir characterization method known as capacitance-resistance model (CRM) for two Mexican fields with highly-complex geology (tight and unconventional). She will infer well connectivity based on to geological characteristics using only the injection and production rates collected from waterflooding.

Results

Agua Fria oil field, located in the Chicontepec Basin in the Gulf of Mexico, is the first asset to be evaluated with the CRM in this project. This deposit of submarine fan turbidite sandstone has a complex geological heterogeneity and variable petrophysical properties across the field. With a long history of water injection (from 2008) and no detailed characterization, this system of intercalated, extremely low-permeability sandstones and shale bodies across the field represents a challenge for reservoir management and a good candidate for CRM application.

A collaborative effort to generate a complete and logical procedure to use the CRM as a reservoir characterization method has been adopted for Agua Fria field to develop a reasonable production-optimization program. Additionally, the CRM results are being taken as support for the geological model generation and its corresponding quality assurance test.

Final remarks

- The CRM results and geological interpretations can be used together to develop a more reliable characterization method for when the reservoir to be analyzed lacks information or is highly complex. In cases when the geological model is in construction, the CRM can be taken as a quality assurance/quality control tool and vice versa.
- For environments as complex as Agua Fria field, the interwell connectivity analysis is a faster and more cost-effective tool for reservoir characterization and decision making. Even though high uncertainty in injection/production data exists, the trend or direction of interwell connectivity found inside the area by the CRM is mostly reliable.
- The accuracy of CRM results can be considered proportional to the injection and production data quality. Less user bias in CRM application will be introduced as the production/injection data uncertainty is reduced.

Integrated fluid characterization and reservoir compartmentalization identification using geochemical techniques

Mengsha Yin
PhD student

Introduction

Mengsha Yin aims to perform an integrated characterization of heavy oil hydrocarbon and non-hydrocarbon fractions and to explain the origins of fluid heterogeneity by combining these data into chemometrics models. The final goal is to assess reservoir connectivity and to configure well placement schemes for rejuvenating production in the study areas.

Results

Mengsha found a novel bicyclic sesquiterpane for assessing middle-level biodegradation. She developed a chemometrics model for the deconvolution of oil biodegradation-mixing history in complex petroleum reservoirs (manuscript under review). Additionally, she estimated the fluid heterogeneity in the studied heavy oil reservoirs by incorporating the molecular composition data into a chemometrics model based on the reservoir geophysical property architecture model achieved by geophysical loggings.

Final remarks

- Biodegradation interacting with oil mixing is the predominant control of heavy oil fluid heterogeneity in heavy oil reservoirs.
- If coupled with whole oil molecular composition data, chemometrics methods are very useful in deciphering the complex oil charging and secondary alteration history.
- The assessment of fluid heterogeneity in heavy oil reservoirs is also necessary for heavy oil recovery along with the geophysical heterogeneity of the reservoir structures, because the data shows greatly-varied fluid compositions between reservoir compartments and, to some extent, even within a single reservoir compartment.

Advanced characterization and innovative solutions for heavy oil recovery in mature fields

Solange Angulo
Research Associate

Introduction

One of the main challenges for the recovery of heavy and extra-heavy oil in mature fields in Mexico is the heterogeneity of the reservoirs and their complex architecture. The field Dr. Solange Angulo, PhD, studies is characterized by barriers and multi-scale compartments that limit the connectivity of the sandstone and consequently, the mobility of the fluids.

The objective of this project is to build an integrated, detailed three-dimensional (3D) model of the reservoir which will be used to optimize the development of the field by using enhanced oil recovery solutions based on steam-solvent-surfactant injection.

Results

The reservoir is characterized by an intercalation of sandstones and mudstones that can be divided into three sedimentary units separated by flooding surfaces, from bottom to top: A, B and C. In terms of the reservoir architecture Unit B is more complex than units A and C, with more localized geobodies, but that might still be interconnected in 3D. In terms of fluids, Unit A and Unit B constitute one flow unit which is oil saturated. In contrast, unit C is more complex, towards the northeast the unit is water saturated, while the rest of the area shows an oil-water contact.

The connectivity of the sand bodies within these sedimentary units was determined based on the recognition of oil-water contacts in the different geobodies interpreted from well log data (gamma ray, resistivity and calculated water saturation). More than 20 geobodies were identified in total.

A 3D model showing the reservoir architecture and the geometry of these geobodies has been built. Once the geobodies are defined, petrophysical properties (such as porosity and water saturation) are modelled using geostatistical techniques. This static 3D model will be used to simulate a pilot test to enhance the recovery of additional volumes of oil from mature heavy oil fields through steam-solvent-surfactant injection.

Final remarks

- The major uncertainties of the 3D model are:
  - Lateral connectivity between geobodies, due to lateral extent of the geobodies.
  - Vertical connectivity between geobodies, due to continuity of mudstone intervals (seals) between geobodies.
  - Oil-water contact location where the actual contact is not observed at well locations.
- The applied geomodeling methodology allows researchers to build several potential distributions of the geobodies, each one capturing a possible geological interpretation, within the limit of the range of uncertainties identified.

Using nanofluids and micro-reservoirs to enhance oil recovery from mature fields in Mexico

Parisa Bazazi
PhD student

Introduction

Nanoparticle dispersions present a revolutionary platform in many applications, including enhanced oil recovery (EOR). Interactions of nanoparticles with the natural surface-active materials in reservoir oil may spontaneously generate new phases in the form of emulsions, alter the liquid-liquid-solid interfacial energies and ultimately affect the fate of EOR's performance. Parisa Bazazi's research aims to characterize and formulate the physiochemical and hydrodynamic properties of nanoparticle dispersion-micellar solution interfaces. She considers the effect of oil phase viscosity and interfacial materials on the dynamics of spontaneous emulsification, drop spreading on solids and oil film detachment from solid surfaces. Parisa's research application is beyond EOR, and can facilitate advances in liquid-in-liquid three-dimensional printing, pesticide spreading and sticking on leaves, and encapsulating drugs in aqueous media.

Results

Parisa found that nanoparticles greatly influence the properties of spontaneously generated emulsions. In systems with low-viscosity oils, submicrometer water droplets nucleate in oil in the form of swollen micelles, forming a microemulsion phase. The gradual surface-activation of nanoparticles by adsorption of surfactants results in the formation of the second type of emulsion from the initially-formed microemulsion, hence, core-shell and multi core-shell emulsions are produced, as shown in Figure 1. She found that the intensity of multiple emulsions strongly depends on the size and concentration of nanoparticles. In systems with higher-viscosity oils, nanoparticles result in the formation of a bicontinuous phase with a lamella structure, shown in Figure 2. In terms of drop spreading, she discovered an unexpected phenomenon whereby the initial spread of drops in the presence of surface-active agents is impeded by the Marangoni stresses, resulting in a large increase in the total spreading time, depicted in Figure 3. Furthermore, her results show that nanoparticles enhance the rate of oil detachment in systems where the oil phase is clean, or it contains a low concentration of surfactants, shown in Figure 4. However, the dynamics of the three-phase contact line remain intact in the presence of nanoparticles when the surrounding oil phase contains a high concentration of surfactants.

Final remarks

- Nanoparticles, under certain conditions, can spontaneously generate multiple emulsions at oil-water interfaces.
- Parisa took advantage of spontaneously-generated bicontinuous phases to develop a new path in forming stable and porous liquid structures by tuning the interplay between the interfacial materials and oil viscosity.
- Parisa engineered the interfacial energies of solid surfaces to fully control the wetting dynamics of solid surfaces by water drops, all submerged in an oil phase. Complete spreading to non-sticking conditions was developed.

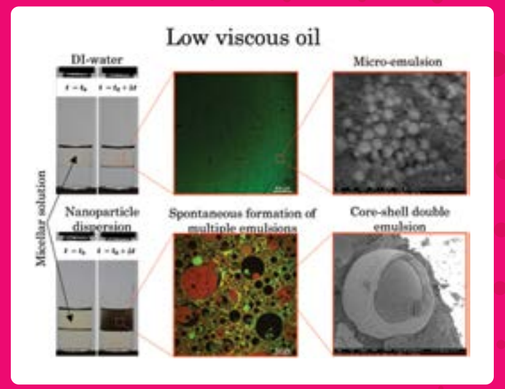


Figure 1

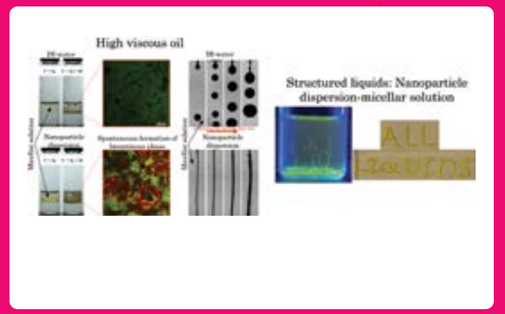


Figure 2

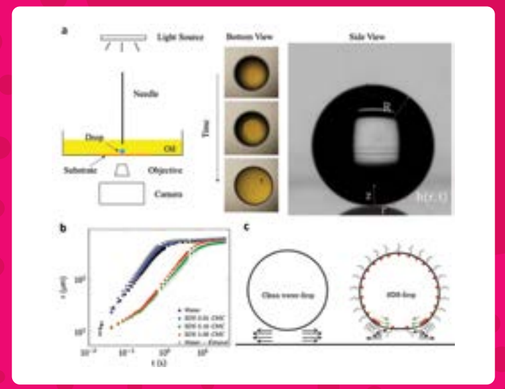


Figure 3

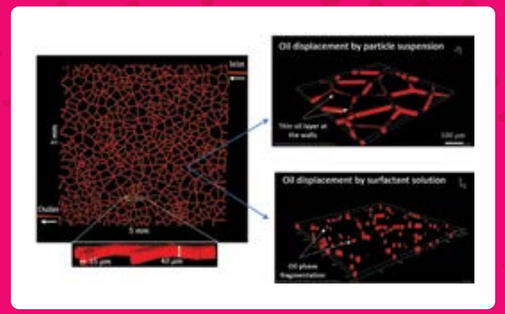


Figure 4

MEXICO RESEARCH COLLABORATION

Using nanofluids and micro-reservoirs to enhance oil recovery from mature fields in Mexico

The interplay between interfacial materials and in situ emulsification for enhanced oil recovery: A visual micromodel study

Hector Bonilla
PhD student

Introduction

Existing studies on flows of particle suspensions in porous media mainly focus on oil recovery in rock samples. Due to the opaque nature of rock structures, the mechanisms underlying the incremental oil recovery have not been fully discovered. In his study, Hector Bonilla developed a visual micromodel resembling the network of pores and throats in a target sandstone rock. The internal surfaces of pores are coated with geomaterials including clays and minerals which enable the interaction of rock-fluid systems. He built an advanced imaging system to record the flow events in the micromodels. The platform is used to study the transport of interfacial materials in terms of surfactants and nanoparticles in the aqueous and oleic phases and their interactions at the oil-water and fluid-solid surfaces. In particular, he investigated the influence of in situ emulsification in the displacement of heavy oil.

Results

Hector used a high pressure-high temperature visual model to enable the study and analysis of the multiple interactions that occur during the oil displacement. His micromodel design is based on a real rock surface, which enables a randomized size and distribution of the pore channels. He found the best combination of particles and surfactants that induce maximum interfacial elasticity, investigated the capability of developed materials in spontaneous emulsification, and performed flooding experiments to discover the performance of generated stable emulsions in oil displacement. The preliminary results demonstrate a considerable increase on the displacement efficiency at the breakthrough of one set of interfacial materials (combined cellulous nanocrystals and surfactants) with that of deionized water.

Final remarks

- Hector developed a new rock-resemble platform for rapid screening of chemical additives for oil recovery.
- He studies in situ oil-in-water emulsification and emulsions flows in porous media.
- The heavy oil displacement by optimized interfacial materials at elevated pressures and temperatures is being investigated.

Using nanofluids and micro-reservoirs to enhance oil recovery from mature fields in Mexico

Residual oil mobilization from EOR studies of unconventional and mature Mexican fields

Mario Cordova Gonzalez
PhD student

Introduction

Mario Cordova Gonzalez's research is to experimentally and numerically investigate strategies to mobilize the remaining oil in mature and waterflooded fields. He uses state-of-the-art research facilities to study the oil-water-solid interactions in microscale visual models based on the pore geometries of a real rock reservoir. Mario first studied the oil-water-chemicals displacement to reveal mechanisms for oil mobilization using integrated flow systems, confocal laser scanning microscopy and micro-particle imaging velocimetry. In parallel, Mario conducted pore-scale numerical simulations of multiphase flows to investigate the balance of viscous and capillary forces which are governing the oil displacement process.

Results

Mario developed an experimental platform to conduct multiphase flow experiments. He investigated the effects of in situ activated nanoparticles in the mobilization of the residual oil. He assessed pore configurations of reservoir rocks using microfluidic chips. Mario used a confocal laser scanning microscope to record the displacement events. He quantified the velocity field in the designed patterns, and the forces exerted on the both phases using a micro-particle-image-velocimetry (micro-PIV) system. Results show that a significant portion of oil remains trapped in dead-end pores and attached to the solid surface. Mario found that there is a notable difference when particles are activated in situ in the displacing fluid compared to in a waterflooding scenario. Mario reproduced the microflow experiments using computational fluid dynamics, solving the mass and momentum conservation equations and reconstructing the interface between the two fluids. Mario's work hints that the precise control and monitoring of pore-scale events and the use of a proper visualization setups provide a strong clarification of the role of chemicals and particles in enhanced oil recovery processes.

Final remarks

- Mario used the microfluidic and computational fluid dynamic approaches to analyze multiphase flow systems in microscale and nanoscale geometries.
- He reports the considerable benefit of in situ activation of particles in desired locations on the oil mobilization from dead-end and bypassed pores.
- He identified mechanisms based on in situ particle activation and spontaneous emulsifications to improve oil recovery from waterflooded porous media.
- His next experiments will track the ex situ bulk emulsification and the in situ formation of emulsion at dynamic displacement events, and introduce flow patterns including flow rate pulses to promote particle and emulsion formations.

GRINSTEM

The University of Calgary through the Global Research Initiative in Sustainable Low Carbon Unconventional Resources (GRI) and with the support of the Canada First Research Excellent Fund (CFREF) has created the GRInstem accelerator program to backup the commercialization of research-intensive innovations within the energy industry and to contribute to the creation of startups. GRInstem projects leverage the expertise of faculty members in chemistry, geosciences and petroleum engineering while creating and testing technologies for future applications in several national and international industries.

The program started in the first quarter of 2019 with two initial enterprises, and rapidly grew to include a total of six HQP-led commercial endeavours that each were awarded $260,000 over a two-year period to support research activities. Additionally, Innovate Calgary provides training, mentorship and support to facilitate the growth of the enterprise.

This section also includes the winners of the Energy Innovators pitch competition, a competition jointly supported by GRI, Innovate Calgary, Hunter Hub for Entrepreneurial Thinking & SAIT. Two teams won $100,000 in in-kind services to help them take their concepts to the next level.

University of Calgary faculty members involved in the projects in this section are Profs. Viola Birss, David Eaton, Ian Gates, Kristopher Innanen, Steve Larter, Roman Shor and Marc Strous.

Novel nanoporous carbon materials for clean water and energy applications

Chengying (Arlene) Ai
Research Assistant

Introduction

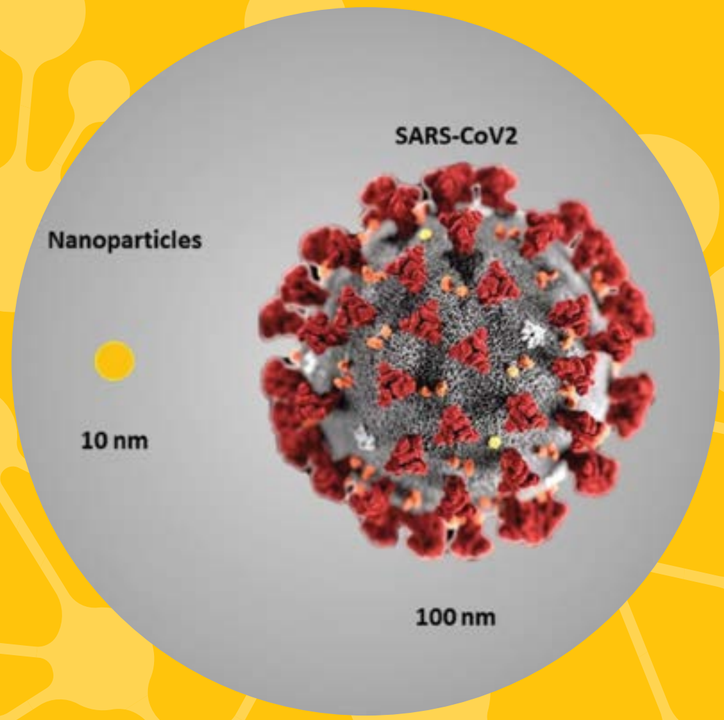
This project is aimed at further improving the existing carbon membrane-based ultrafiltration technology, scaling it up and commercializing it. Arlene Ai's current goal is to understand the market. She is working alongside Dr. Anand Singh, who is helping further develop the technology to meet industrial needs. The carbon membrane being studied was originally developed in Dr. Viola Birss' Group in the Department of Chemistry at the University of Calgary. It is unique in that it contains a fully-tunable network of three-dimensionally interconnected pores, and it is conducting and scalable. Its good heat and chemical resistance make it very promising in ultrafiltration applications under challenging conditions, such as high temperature, acid or caustic chemical filtrations.

Results

Arlene has identified an existing challenge associated with present-day technologies related to membrane fouling through primary market research. The global ultrafiltration membrane market is projected to be worth $4.5 billion by 2021. It is a large market, but there are still some gaps. Fouling is one of the gaps for which many industries are seeking solutions. Arlene and her co-workers found that by applying electrical pulses, the membrane could be cleaned in place at an efficiency of 70 per cent. This means a 70 per cent reduction in chemicals or water used for membrane cleaning. This finding has been filed for a U.S. provisional patent. Arlene's results show that the carbon membrane rejects 100 per cent of spherical nanoparticles with a 10 nanometre diameter, which is significantly smaller than the SARS-CoV2 virus, making virus filtration from gases or liquids another possible application of the membrane.

Final remarks

- Arlene concluded that the carbon membrane can be regenerated by up to 70 per cent through the application of electrical pulses.
- Her next step is to optimize the membrane-cleaning efficiency by tuning the conditions used or combining with other membrane cleaning methods.
- Arlene also concluded that the carbon membrane could be a market changer because of its good chemical and heat resistance and electrical conductivity.
- Dr. Anand Singh is providing significant help in terms of further lab testing and the carbon membrane optimization to fit market needs and demonstration of the carbon membrane capabilities in the filtration area.
- Arlene and Dr. Viola Birss believe that the carbon membrane could potentially be used to remove SARS-CoV2 virus from various fluids, and are currently seeking collaborators to verify this.
- A provisional patent has been filed on Filtration Using Nanoporous Carbon Membranes.



GRINSTEM

LysisLogic Scientific Inc.

Renzo Correa Silva
Research Associate

Introduction

Dr. Renzo Correa Silva, PhD, is the co-founder and CEO of LysisLogic Scientific Inc., and through the GRInstem grant has been working to enable a series of high-risk high-reward innovation projects spanning advanced petroleum system tools to novel materials out of petroleum industry by-products and from climate change mitigation moonshots to chemical database intelligence applied to consumer products. In this project, beyond the value proposition in each research sub-project, Renzo endeavours to develop an innovation nursery model that is suitable for a pragmatic but creative approach to test science-based business hypotheses while focusing on the generation of intellectual property and commercialization.

Results

Regarding petroleum exploration tools, Renzo has expanded the number of case studies tested under one of his inventions — petroleum fluid residence time measurements, arguably the Higgs boson of petroleum geochemistry — and a U.S. patent has been filed. The team has extensively explored climate change mitigation routes involving large-scale facilities and the sequestration of carbon in the ocean ecosystem, and a pivot towards the inorganic carbon pool is currently underway, with new partners on board. New sulphur-based materials for energy storage and other applications are being synthesized in the lab. Renzo is also co-leading an innovation-focused, lab-based initiative that will help impactful ideas meet the necessary lab resources to become an innovation.

Final remarks

- There is much value to extract from impactful ideas that often never find the necessary laboratory resources to be fully scoped and tested. Renzo has been working to bridge such a gap within academia and LysisLogic Inc.
- A moonshot research project involving electrochemistry and inorganic carbon sequestration in oceans has been scoped and hypothesis-testing experiments are underway.
- Renzo's lab is set to synthesize a whole range of sulphur-based polymeric materials.
- Under the petroleum-system tools umbrella, the team has focused on making the technical achievements reachable, via patents and publications, to a larger audience.
- The company has been successful in securing its first sale.

Geophysical imaging and full-waveform inversion while drilling

Nasser Kazemi
Postdoctoral Fellow

Introduction

Dr. Nasser Kazemi, PhD, works on seismic imaging and full-waveform inversion (FWI) of oil and gas reservoirs. The goal of the project is to reduce the environmental footprints and improve the productivity of seismic exploration and exploitation of reservoirs. To do so, Nasser integrates seismic and seismic-while-drilling (SWD) imaging with the development and production workflows. To deliver the project, he uses several tools such as seismic signal processing, machine learning, seismic imaging, full-waveform inversion and drill string dynamics optimization. He received the GRInstem fellowship to commercialize his research findings. Also, he filed a provisional patent on the FWI of the seismic-while-drilling dataset.

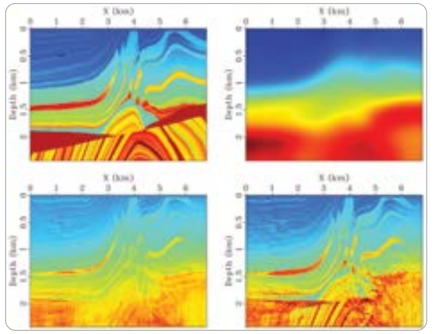


Figure 1

Results

Nasser developed depth imaging and the FWI of the seismic-while-drilling dataset to address the uncertainties of sub-surface imaging in surface seismic. Surface seismic suffers from non-uniform sub-surface illumination and a lack of low-frequency content. Accordingly, depth imaging and FWI struggle to provide accurate subsurface properties. To remedy this shortcoming, he uses SWD data to reduce the uncertainties of sub-surface imaging. SWD imaging overlaid on a detailed McMurray velocity model illustrates that the method successfully images the sub-surface. In another complex sub-surface example, he shows that after using the SWD data, the physical properties of the sub-surface are accurately imaged, Figure1-lower right, compared to that of surface seismic FWI, Figure1-lower left. The ground-truth sub-surface model is shown in Figure1-upper left, and the smooth initial estimate of the sub-surface model provided by kinematic analysis of the pre-stack surface seismic data is represented in Figure1-upper right.

Final remarks

- Seismic data provides an opportunity to build a physically plausible and realistic sub-surface model that honors the geology.
- Sub-surface images provided by processing surface seismic data suffer from non-uniform illumination.
- Seismic-while-drilling imaging and FWI show promise in improving the resolution of sub-surface images.
- Reducing the uncertainties of subsurface images improves well placement and production plans.
- The developed workflow provides the necessary tools for reducing the seismic acquisition footprints and improving the productivity of oil and gas reservoirs.

ASEISMIC Solutions Inc.

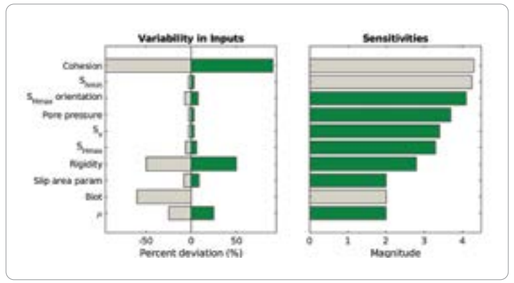
Thomas Eyre and David Eaton

Awards received

- GRInstem
- Energy Innovators

ASEISMIC Solutions Inc. provides an integrative solution for modelling and mitigating induced seismicity. Induced earthquakes are a known hazard for anthropogenic activities such as hydraulic fracturing and carbon dioxide sequestration. They can lead to significant financial impacts for operators, and potentially damage local structures and infrastructure. Efforts to quantify induced-seismicity risk and to develop mitigation strategies are hampered by a lack of numerical schemes that can accommodate realistic earth models while capturing the full spectrum of applicable physics.

By combining reservoir simulation methods with advanced geomechanical and seismological computational tools, ASEISMIC Solutions Inc. is developing a new computational toolbox to aid in generating quantitative mitigation and response strategies. The toolbox includes modules for site-specific induced-seismicity operational risk assessment based on augmenting relevant public data sources with additional site-specific information. It takes a probabilistic approach to account for the inherent uncertainties in this type of modelling. Case studies from Western Canada are used to evaluate the applicability of this approach for unconventional oil and gas development and other applications such as gigaton-scale carbon dioxide storage. Ultimately, the software aims to significantly reduce the financial, environmental and social risk of induced seismicity.



CElect Technologies — Solid Polymer Electrolyte CO_2 Electrolyzers

Parisa (Fatemeh) Karimi, Amir Alihosseinzadeh and Josh Koenig

Awards received

- Energy Innovators

The team is working on developing a novel, efficient and easily-scalable electrochemical reactor to convert CO_2, water and renewable electricity to value-added chemicals. Their reactor has many advantages including:

- Increased compactness
- Room temperature operation
- Cheaper balance of plant
- Faster response
- No need for corrosive liquid electrolyte
- Less product contamination
- Better long-term stability
- Design based on polymer electrolyte reactors widely used in industrial scales

Earth Impulse Solutions Ltd.

Nasser Kazemi Nojadeh, Roman Shor, Kristopher Innanen and Ian Gates

Awards received

- GRInstem


Dr. Nasser Kazemi


Dr. Roman Shor


Dr. Kris Innanen


Dr. Ian Gates

Earth Impulse is a signal processing and imaging company that provides optimal solutions for sub-surface imaging before and while drilling, efficient drilling and well placement, and development and production of complex oil/gas reservoirs. Earth impulse is co-founded by Dr. Nasser Kazemi, Director and CEO, Dr. Roman Shor, Director, Dr. Kristopher Innanen, Director, and Dr. Ian Gates, Director. The directors of Earth Impulse have extensive industry and research experience in geophysical seismic processing and imaging, drilling control and optimization, and reservoir characterization. After two and half years of solid research on improving the efficiency of drilling practices and sub-surface imaging, the inventors, Nasser, Roman and Kristopher, filed a provisional patent on full-waveform inversion and sub-surface imaging by using surface seismic and seismic-while-drilling technology. Earth Impulse has established a partnership with Innovate Calgary to take advantage of their long-lasting experiences in commercialization and attracting interested investors.

The company has developed a working prototype and a lab-scale trial. The dynamic team of researchers and software developers is working tirelessly to provide solutions that increase the efficiency and productivity of oil/gas reservoirs without interrupting the routine practices of the oil and gas industry. Several publications in high impact journals such as *Society of Petroleum Engineers* journals, *Geophysics*, and *Institute of Electrical and Electronics Engineers* journals show the added value and innovative nature of the technology developed by the team.

ForScent Inc.

Ranjani Kannaiyan, Jingyi (Jacky) Wang and Ian Gates

Awards received

- GRInstem

ForScent is a spin-off company from the University of Calgary from the GRI program which has solutions for the reduction of odor in oil sands and petroleum processing plants. ForScent's technology will reduce sulphur-compound-caused odors so that the impact of odor on communities that are close to oil and gas operating sites is reduced or eliminated. For communities adjacent or near oil and gas processing facilities, for example oil sands plants and oil processing batteries, emissions from the operations can lead to strong odors which can impact people's lives.

The odor problem near these operating facilities has been a recurrent issue for communities for many years and many of the most odorous materials are sulphur-based compounds. The team intends on testing and verifying their technology using gas chambers with field testing trials in late 2021. The team for this GRInstem company consists of Ranjani Kannaiyan (CEO), Jingyi (Jacky) Wang (CTO), and Ian Gates (COO).

LysisLogic Scientific Inc.

Renzo Correa Silva, Jagos Radovic and Steve Larter

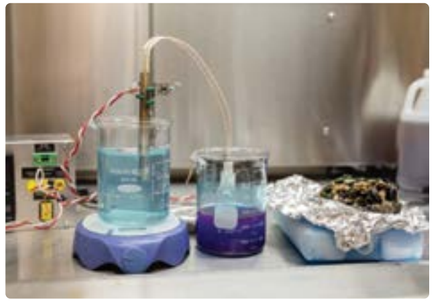
Awards received

- GRInstem

LysisLogic Inc. thrives on developing technologies from natural or human-made processes that impact organic matter and occur over short or geological time scales. This is done through analysis, modelling, experimental design and creative thinking. While developing advanced petroleum system tools to make the exploration of unconventional resources more efficient, the company also nurtures early-stage technologies for the transitioning energy industry and value-added consumer products. The team has a combination of diverse experience in both academia and industry, and the curiosity and pragmatism to develop useful solutions to the challenges at hand. Within LysisLogic and its multi-pronged startup-like structure, the team has a unique opportunity to nurture applied research and offer their expertise in organic matter transformation for a broader audience. They have two main solution streams:

Advanced Petroleum System Tools

Designed to assist businesses in their quest for optimized petroleum exploration, in this stream, proprietary technology and a modelling software tool enable new insights and measurements relating to the complexities of petroleum charge and alteration.



Innovation nursery

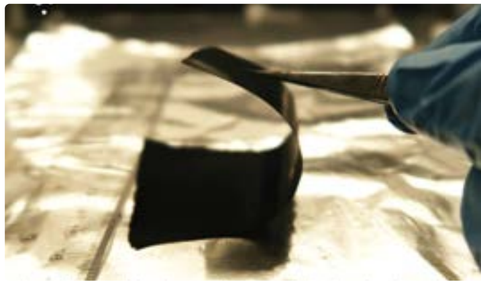
Here, with partners at UCalgary, LysisLogic Inc. focuses on a range of high impact opportunities, including novel polymers from fossil fuel industry by-products, ocean-based large-scale climate change mitigation strategies and novel complex-mixture chemical processes focused on consumer products.

Momentum Materials Solutions Corp.

Chengying (Arlene) Ai, Anand Singh and Viola Birss

Awards received

- GRInstem



Membrane filtration is a critical process in a wide scope of industries, including the pharmaceutical, chemical and petrochemical industries. This represents a $3 billion global market. However, membranes foul easily and have to be cleaned frequently by either chemical washing or back flushing, which consumes a large amount of chemicals or water. Defouling could increase the operation cost by 50 to 100 per cent. Hence, there is a significant need and market for fouling tolerant membranes.

Momentum Materials Solutions is developing a membrane filtration technology based on a patented nanoporous carbon membrane. The carbon membrane has excellent conductivity, exquisitely tunable porosity and related nanoproperties, and outstanding thermal and chemical resistance. Another unique feature is that it can be cleaned in place simply by applying periodic electrical pulses to split water. This generates gas bubbles that dislodge any clogging solids from the membrane surface, making the process highly efficient, cost-effective and straightforward. The removed foulants can then be washed away with the feed solution to the side flow, thus eliminating up to 70 per cent of the chemicals and water normally used for membrane recovery while also minimizing liquid discharge and lowering operation costs by 50 per cent as compared to other commercial membranes.

The Momentum Materials Solutions team includes Chengying (Arlene) Ai (co-founder and CEO), Dr. Anand Singh (vice-president of research and development) and Dr. Viola Birss (co-founder and Scientific Director). Momentum Materials Solutions is seeking potential customers and strategic collaborators to validate the technology.

Synergia Biotech Inc.

Agasteswar Vadlamani, Marc Strous and Angela Kouris

Awards received

- GRInstem

Synergia Biotech has created a completely natural, carbon-negative blue-colour ingredient using a patent-pending bioprocess. The lower-cost, high purity phycocyanin is released from cyanobacteria that use carbon dioxide sourced from clean air. Artificial colours are well on their way to extinction because they cause hyperactivity in children, allergenicity and toxicity. Synergia Biotech's new "green" blue can replace chemical colouring additives in the food and beverage, health and wellness, and personal care industries.

Synergia Biotech's innovations in process ecology, biomass dewatering and phycocyanin separation lead to very low energy consumption, enable recycling of process water and drive climate benefits. Ten per cent of the captured CO_2 is converted to high-value phycocyanin, and the remainder to zero-carbon natural gas.

Federally incorporated in 2019, Synergia Biotech graduated from the Creative Destruction Lab, a highly competitive, objective-based business accelerator program in June 2020. In addition to gaining a network of trusted business mentors and fellow innovators, they received ten offers for financing meetings from CDL Fellows and Associates. They have received expressions of interest from two of the top three global natural colour companies to evaluate their product and have engaged a leading food industry development centre to develop formulations for food and beverage applications.

Synergia has scaled up from the benchtop model to a pre-commercial pilot plant and plans to further scale and de-risk the technology. The product and the market at a commercial level are underway. Synergia Biotech anticipates being the world's leading phycocyanin producer while operating hectares of raceway ponds globally within ten years.

The team includes Angela Kouris (CEO & Co-founder), Agasteswar Vadlamani (CTO & Co-founder), Christine Sharpe (Director & Co-founder), Marc Strous (Director & Co-founder) and Benjamin Lightburn (Director, Chief Business Strategist).

GRADUATED HQP

MSc

Jason Matthew Abboud
Thesis Title: *"In situ free phase gas production in initially saturated sediment"*
http://hdl.handle.net/1880/110213

Orrsam Aadil Abubaker
Thesis Title: *"Perovskite-type cathode material for intermediate temperature solid oxide fuel cells"*
http://hdl.handle.net/1880/112106

Maysam Alnajjar
Thesis Title: *"Preparation and application of amorphous silica-alumina for the removal of pharmaceutical compounds from water"*
http://hdl.handle.net/1880/109447

Alexander Bradley
Thesis Title: *"Investigating the environmental impacts of Western Canadian tight oil resources"*
http://hdl.handle.net/1880/111763

Maria Caceres Falla
Thesis Title: *"Integrating direct air carbon capture and microalgae-based bioenergy production"*
http://hdl.handle.net/1880/111614

Karen Canon-Rubio
Thesis Title: *"Strategies for improving the productivity and cost-effectiveness of microalgal production systems"*
http://hdl.handle.net/11023/2902

Emilio Cavanzo Balcazar
Thesis Title: *"Solvent diffusion in a solvent/water/bitumen system"*
https://prism.ucalgary.ca/handle/1880/111766

Juliann Coffey
Thesis Title: *"Characterization of the Southern Rocky Mountain Trench near Valemount, British Columbia, using receiver functions"*
http://hdl.handle.net/1880/112119

Ali Farhangfar
Thesis Title: *"LPV gain scheduling control for variable speed variable pitch wind turbines"* http://hdl.handle.net/11023/4142

Muhammad Fowaz Ikram
Thesis Title: *"Effective thermal properties of granular porous media: a numerical study using Lattice Blotzmann Methods"*
http://hdl.handle.net/1880/106253

Adriana Gordon
Thesis Title: *"Processing of DAS and geophone VSP data from the CaMI Field Research Station"*
https://prism.ucalgary.ca/handle/1880/110175

Joshua Heidebrecht
Thesis Title: *"Ligand design for energy conversion and storage applications"*
http://hdl.handle.net/1880/111355

Xuemin Huang
Thesis Title: *"Application of Dilation-Recompaction Model in hydraulic fracturing simulation"*
http://hdl.handle.net/11023/2199

Heidi Jahandideh
Thesis Title: *"The role of graphene oxide — polyacrylamide interactions on the stability and microstructure of oil-in-water emulsions"*
http://hdl.handle.net/1880/107701

Kushagra Kakar
Thesis Title: *"Artificial neural network modeling of well performance in the Garrington Field, Cardium Formation"*
http://hdl.handle.net/1880/109399

Gaurav Kumar
Thesis Title: *"Settling dynamics of two spheres in a diluted suspension of brownian rods"*
http://hdl.handle.net/1880/110778

Mozhu Li
Thesis Title: *"Phosphorus recovery from synthetic municipal wastewater through lignin-induced struvite precipitation"*
http://hdl.handle.net/1880/111494

Xiaoying Li
Thesis Title: *"Comprehensive performance optimization of a water-alternating-carbon-dioxide reservoir"*
http://hdl.handle.net/1880/106589

Jialang (Christine) Li
Thesis Title: *"Cell design and electrode material for all vanadium redox flow battery"*
http://hdl.handle.net/1880/106432

Omar Maan
Thesis Title: *"Development of polyacrylamide composite hydrogel for removal of humic acid based on interaction studies"*
http://hdl.handle.net/1880/108776

Rachel Malone
Thesis Title: *"A confocal rheology study of network stabilized bicontinuous emulsion gels"*
http://hdl.handle.net/1880/107684

Nedal Marei
Thesis Title: *"Role of nanosize effects on the adsorptive and catalytic properties of nio nanoparticles towards heavy hydrocarbons"*
http://hdl.handle.net/11023/2974

Aseem Pandey
Thesis Title: *"Microstructure and flow behavior of cellulose nanocrystal stabilized emulsions with repulsive and attractive interactions"*
https://prism.ucalgary.ca/handle/1880/109369

Josh Purba
Thesis Title: *"Seismicity and tectonic interpretation of the Southern Rocky Mountain Trench near Valemount, British Columbia, Canada"*
http://hdl.handle.net/1880/112078

Tyler Spackman
Thesis Title: *"Novel orbital seismic sources at a CO_2 storage monitoring site, Newell County, Alberta"*
http://hdl.handle.net/1880/110245

Safina Ujan
Thesis Title: *"Towards the optimization of lipid and antioxidant production in microalgae: A metabolic stud"*
http://hdl.handle.net/1880/111572

Volodymer Vragov
Thesis Title: *"Comparison of convolutional neural networks with matched-filtering for detection of induced seismicity"*
http://hdl.handle.net/1880/110751

Miao Wang
Thesis Title: *"Comparative techno-economic analysis of ammonia electrosynthesis"*
http://hdl.handle.net/1880/111617

Yecan Wang
Thesis Title: *"Dendrimer functionalized nanocrystalline cellulose for environmental applications"*
http://hdl.handle.net/1880/111526

Min Wang
Thesis Title: *"Enhancing hydrocarbon recovery and sensitivity studies in tight liquid-rich gas resources"*
http://hdl.handle.net/11023/3850

Calista Yim
Thesis Title: *"Organic sulfur-bearing species as subsurface carbon storage vectors"*
https://prism.ucalgary.ca/handle/1880/110919

PhD

Paul Addo
Thesis Title: *"Development of fuel electrodes for reversible solid oxide fuel cell applications"*
http://hdl.handle.net/11023/3735

Maureen Austin-Adigio
Thesis Title: *"Enhancing Steam-Assisted Gravity Drainage applications in challenging and non-challenging oil sands reservoirs"*
http://hdl.handle.net/1880/107634

Raul Cova Gamero
Thesis Title: *"Near-surface S-wave traveltime corrections and inversion: a raypath-consistent and interferometric approach"*
http://hdl.handle.net/11023/4081

Abdallah Darweesh Manasrah
Thesis Title: *"Conversion of petroleum coke into valuable products using catalytic and non-catalytic oxy-cracking reaction"*
http://hdl.handle.net/1880/106532

Sajjad Esmaeili
Thesis Title: *"Effect of temperature on two-phase oil/water relative permeability under sagd conditions"*
http://hdl.handle.net/1880/112232

Seyed Mostafa Jafari Raad
Thesis Title: *"Buoyancy driven flows in porous media with applications to geological storage of carbon dioxide"*
http://hdl.handle.net/1880/110179

Aprami Jaggi
Thesis Title: *"Dissolved organic matter in marine environments: a study of the origin, lability and molecular composition"*
http://hdl.handle.net/1880/106479

Suzie Jia
Thesis Title: *"Stress inversion and damage quantification in tight gas shale with application to hydraulic fracturing"*
http://hdl.handle.net/1880/111214

Bing Kong
Thesis Title: *"Production analysis and enhancement in the unconventional tight formations"*
http://hdl.handle.net/1880/111449

Junxiao Li
Thesis Title: *"Borehole wave field modeling, reflection extraction and reverse time migration in acoustic reflection imaging logging"*
http://hdl.handle.net/1880/106213

Qi Li
Thesis Title: *"Microseismic based reservoir characterization (sbrc): stimulated reservoir volume, diffusivity, geomechanics and probabilistic modeling"*
http://hdl.handle.net/1880/106596

Ran Li
Thesis Title: *"Multi-scale gas flow in shale pores with water films"*
http://hdl.handle.net/1880/110532

Mason MacKay
Thesis Title: *"Rock mass characterisation and the hydro-mechanical behaviour within interbedded low permeability reservoirs during hydraulic fracturing"*
http://hdl.handle.net/1880/109198

Peyman Mohammadmoradi
Thesis Title: *"Pore morphological multi-phase digital rock physics models"*
http://hdl.handle.net/11023/3485

Beatriz Molero Sanchez
Thesis Title: *"Development of oxygen electrodes for reversible solid oxide fuel cells"*
http://hdl.handle.net/11023/3833

Mehrshad Parchei Esfahani
Thesis Title: *"Kinetic and mass transfer of peroxone oxidation of toluene using ultra sonic spray: ab initio quantum calculations and numerical modeling"*
http://hdl.handle.net/1880/111512

Helen Pinto
Thesis Title: *"Insights on the thermal efficiency of SAGD from data analytics"*
http://hdl.handle.net/1880/111643

Will Richardson
Thesis Title: *"Diffusivity of light hydrocarbon gases in bitumen"*
http://hdl.handle.net/11023/3742

German Rodriguez-Pradilla
Thesis Title: *"Microseismic monitoring of a Duvernay Hydraulic-Fracturing Stimulation, Alberta Canada: Processing and interpretation assisted by finite-difference synthetic seismograms"*
https://prism.ucalgary.ca/handle/1880/111335

Mahta Sadeghvishka
Thesis Title: *"Modelling of geomechanics for informed hydraulic fracturing operations"*
http://hdl.handle.net/11023/4109

Farbod Sharif
Thesis Title: *"Water treatment by adsorption with electrochemical regeneration using graphene-based materials"*
http://hdl.handle.net/1880/106319

Navreet Kaur Suri
Thesis Title: *"Microbially-enhanced oil recovery through activity of alkylbenzene-oxidizing nitrate-reducing bacteria"*
http://hdl.handle.net/11023/4176

Evar Chinedu Umeozor
Thesis Title: *"Energy and emissions of unconventional resources"*
http://hdl.handle.net/1880/109461

Shuhua Wang
Thesis Title: *"Integrated data mining and optimization in hydraulic fractured tight oil reservoirs"*
http://hdl.handle.net/1880/106614

Thomas Welsh
Thesis Title: *"Direct (Hetero) arylation for the efficient synthesis of ϖ-conjugated materials for use in organic electronics"*
http://hdl.handle.net/1880/110941

Norman Wong
Thesis Title: *"Tuning proton conduction in metal-organic frameworks"*
http://hdl.handle.net/11023/3951

Chongchong Wu
Thesis Title: *"Computational study on removal of naphthenic acids from petroleum-based systems"*
http://hdl.handle.net/1880/106332

Bo Yang
Thesis Title: *"Preconditioned iterative solvers on GPU and an in-situ combustion simulator"*
http://hdl.handle.net/1880/111505

Jie (Jason) Zhan
Thesis Title: *"Multi-scale numerical studies on characterization of shale gas reservoir development"*
http://hdl.handle.net/1880/106660

Yaqi Zhang
"Geomaterial-functionalized microfluidic devices for multiphase flow in porous media"
http://hdl.handle.net/1880/111

Postdoctoral Fellows

Huaizhen Chen
Project Title: *"Azimuthal seismic inversion for new indicators of oil-bearing fractured reservoirs"*

Xiaoli Dong
Project Title: *"Robust, high-productivity phototrophic carbon capture at high ph and alkalinity using natural microbial communities"*

Ruimin Feng
Project Title: *"Crack initiation characteristics of gas-containing coal under gas pressures"*

Pauline Humez
Project Title*: "The contribution of aqueous catechol-silica complexes to silicification during carbonate diagenesis"*

Marie Macquet
Project Title: *"A feasibility study for detection thresholds of CO2 at shallow depths at the CaMI Field Research Station, Newell County, Alberta, Canada"*

Arpita Nandy
Project Title: *"Comparative evaluation of coated and non-coated carbon electrodes in a microbial fuel cell for treatment of municipal sludge"*

Abdolmohsen Shabib-Asl
Project Title: *"Evaluation and manipulation of the fundamental controls on hydrocarbon fluid recovery and GHG storage using Ghgs as the injected fluid"*

Christine Elizabeth Sharp
Project Title: *"Robust, high-productivity phototrophic carbon capture at high ph and alkalinity using natural microbial communities"*

Kalpana Singh
Project Title: *"Engineering and developing advanced cathodes for proton conducting solid oxide fuel cells using electrochemical impedance spectroscopy genetic programming"*

Ping Song
Project Title: *"Interfacial property of metal organic frameworks for oil recovery, oil/water separation, and water treatment*

PUBLICATIONS

Peer-reviewed journal articles

Abubaker, O. A., Singh, K., & Thangadurai, V. (2020). Investigating the effect of Cu-doping on the electrochemical properties of perovskite-type Ba0.5Sr0.5Fe1-xCuxO3-δ (0≤ x≤ 0.20) cathodes. *Journal of Power Sources,* 451, 227777.

Auriol, J., Aarsnes, U. J. F., Di Meglio, F., & Shor, R. (2020). Robust Control Design of Underactuated 2× 2 PDE-ODE-PDE Systems. *IEEE Control Systems Letters,* 5(2), 469-474.

Auriol, J., Shor, R. J., Aarsnes, U. J. F., & Di Meglio, F. (2020). Closed-loop tool face control with the bit off-bottom. *Journal of Process Control,* 90, 35-45.

Chang, Q., Zhang, P., Mostaghimi, A. H. B., Zhao, X., Denny, S. R., Lee, J. H., Gao, H., Zhang, Y., Xin, H. L., Siahrostami, S., Chen, J. G., & Chen, Z. (2020). Promoting H_2O_2 production via 2-electron oxygen reduction by coordinating partially oxidized Pd with defect carbon. *Nature Communications*, 11(1), 1-9.

Chen, H., Chen, T., & Innanen, K. A. (2020). Estimating tilted fracture weaknesses from azimuthal differences in seismic amplitude data. *Geophysics, 85*(3), R135-R146.

Chen, H., Li, J., & Innanen, K. A. (2020). Nonlinear inversion of seismic amplitude variation with offset for an effective stress parameter. *Geophysics, 85(4)*, R299-R311.

Culbertson, C. M., Flak, A. T., Yatskin, M., Cheong, P. H. Y., Cann, D. P., & Dolgos, M. R. (2020). Neutron total scattering studies of group II titanates (ATiO3, A2+= Mg, Ca, Sr, Ba). *Scientific Reports, 10(1)*, 1-10.

DiCaprio, L., Maiti, T., Dettmer, J., & Eaton, D. W. (2020). Moho structure across the Backarc-Craton transition in the Northern US Cordillera. *Tectonics, 39*(2), e2019TC005489.

Eyre, T. S., Zecevic, M., Salvage, R. O., & Eaton, D. W. (2020). A Long-Lived Swarm of Hydraulic Fracturing-Induced Seismicity Provides Evidence for Aseismic Slip. *Bulletin of the Seismological Society of America.*

Esmaeili, S., Sarma, H., Harding, T., & Maini, B. (2020). Experimental study of the effect of solvent addition and temperature on two-phase bitumen/water relative permeability. *SPE Reservoir Evaluation & Engineering.*

Esmaeili, S., Modaresghazani, J., Sarma, H., Harding, T., & Maini, B. (2020). Effect of temperature on relative permeability–Role of viscosity ratio. *Fuel, 278,* 118318.

Gao, Z., Xu, S., Li, L., Yan, G., Yang, W., Wu, C., & Gates, I. D. (2020). On the adsorption of elemental mercury on single-atom TM (TM= V, Cr, Mn, Co) decorated graphene substrates. *Applied Surface Science,* 146037.

Gibbons, B. M., Wette, M., Stevens, M. B., Davis, R. C., Siahrostami, S., Kreider, M., Mehta, A., Higgins, D. C., Clemens, B. M, & Jaramillo, T. F. (2020). In situ X-ray absorption spectroscopy disentangles the roles of copper and silver in a bimetallic catalyst for the oxygen reduction reaction. *Chemistry of Materials, 32*(5), 1819-1827.

Gusarov, S., Stoyanov, S. R., & Siahrostami, S. (2020). Development of Fukui Function Based Descriptors for a Machine Learning Study of CO_2 Reduction. *The Journal of Physical Chemistry C, 124*(18), 10079-10084.

Han, G. F., Li, F., Zou, W., Karamad, M., Jeon, J. P., Kim, S. W., Kim, S. J., Bu, Y., Fu, Z., Lu, Y., Siahrostami, S., & Baek, J. B. (2020). Building and identifying highly active oxygenated groups in carbon materials for oxygen reduction to H_2O_2. *Nature Communications, 11*(1), 1-9.

Hannouf, M., Assefa, G., & Gates, I. (2020). From social hotspots to policies for successful implementation of environmentally better technologies? The example of social life cycle assessment of oil and gas technologies in Alberta, Canada. *Environmental Science & Policy, 110,* 24-33.

Hosseini, E., Kollath, V. O., & Karan, K. (2020). The key mechanism of conductivity in PEDOT: PSS thin films exposed by anomalous conduction behaviour upon solvent-doping and sulfuric acid post-treatment. *Journal of Materials Chemistry C, 8*(12), 3982-3990.

Hosseini, E., Arjmand, M., Sundararaj, U., & Karan, K. (2020). Filler-free conducting polymers as a new class of transparent electromagnetic interference shields. *ACS Applied Materials & Interfaces.*

Huang, X., & Gates, I. (2020). Apparent contact angle around the periphery of a liquid drop on roughened surfaces. *Scientific Reports, 10*(1), 1-11.

Kammampata, S. P., Yamada, H., Ito, T., Paul, R., & Thangadurai, V. (2020). The activation entropy for ionic conduction and critical current density for Li charge transfer in novel garnet-type $Li_{6.5}La_{2.9}A_{0.1}Zr_{1.4}Ta_{0.6}O_{12}$ (A= Ca, Sr, Ba) solid electrolytes. *Journal of Materials Chemistry A, 8*(5), 2581-2590.

Khot, V., Strous, M., & Hawley, A. K. (2020). Computational approaches in viral ecology. *Computational and Structural Biotechnology Journal, 18*, 1605-1612.

Koenig, J. D., Farahat, M. E., Dhindsa, J. S., Gilroy, J. B., & Welch, G. C. (2020). Near-IR absorption and photocurrent generation using a first-of-its-kind boron difluoride formazanate non-fullerene acceptor. *Materials Chemistry Frontiers, 4,* 1643-1647.

Li, Z., Wang, J., & Gates, I. D. (2020). Fracturing Gels as Analogs to Understand Fracture Behavior in Shale Gas Reservoirs. *Rock Mechanics and Rock Engineering.*

Li, S., & Du, K. (2020). Comparisons of forward-in-time and backward-in-time Lagrangian stochastic dispersion models for micro-scale atmospheric dispersion. *Journal of the Air & Waste Management Association, 70*(4), 425-435.

Li, Z., Huang, H., & Zhang, S. (2020). The effect of biodegradation on bound biomarkers released from intermediate-temperature gold-tube pyrolysis of severely biodegraded Athabasca bitumen. *Fuel, 263,* 116669.

Liu, C. M., Sandhu, N. K., McCoy, S. T., & Bergerson, J. A. (2020). A life cycle assessment of greenhouse gas emissions from direct air capture and Fischer–Tropsch fuel production. *Sustainable Energy & Fuels, 4,* 3129-3142.

Ma, Y., Ardakani, O. H., Zhong, N., Liu, H., Huang, H., Larter, S., & Zhang, C. (2020). Possible pore structure deformation effects on the shale gas enrichment: an example from the Lower Cambrian shales of the Eastern Upper Yangtze Platform, South China. *International Journal of Coal Geology, 217,* 103349.

Ma, Y., Zhong, N., Yao, L., Huang, H., Larter, S., & Jiao, W. (2020). Shale gas desorption behavior and carbon isotopic variations of gases from canister desorption of two sets of gas shales in south China. *Marine and Petroleum Geology, 113,* 104127.

Mainville, M., Tremblay, V., Fenniri, M. Z., Laventure, A., Farahat, M. E., Ambrose, R., Welch, G. C., Hill, I. G. & Leclerc, M. (2020) Water compatible direct (hetero) arylation polymerization of PPDT2FBT: A pathway towards large-scale production of organic solar cells. *Asian Journal of Organic Chemistry, 9,* 1-9.

Manasrah, A. D, G. Vitale and N. N. Nassar (2020) Catalytic oxy-cracking of petroleum coke on copper silicate for production of humic acids. *Applied Catalysis B: Environmental,* 118472.

Mohsin, I., Al-Attas, T. A., Sumon, K. Z., Bergerson, J., McCoy, S., & Kibria, M. G. (2020). Economic and environmental assessment of integrated carbon capture and utilization. *Cell Reports Physical Science, 1*(7) 100104.

Mostaghimi, A. H. B., Al-Attas, T. A., Kibria, M. G., & Siahrostami, S. (2020). A review on electrocatalytic oxidation of methane to oxygenates. *Journal of Materials Chemistry A.*

Moud, A. A., Kamkar, M., Sanati-Nezhad, A., Hejazi, S. H., & Sundararaj, U. (2020). Nonlinear viscoelastic characterization of charged cellulose nanocrystal network structure in the presence of salt in aqueous media. *Cellulose, 27*(10), 5729-5743.

Mulmi, S., & Thangadurai, V. (2020). Editors' Choice-Review-Solid-state electrochemical carbon dioxide sensors: fundamentals, materials and applications. *Journal of the Electrochemical Society, 167*(3), 037567.

Nagarajan, B., Kamkar, M., Schoen, M. A., Sundararaj, U., Trudel, S., Qureshi, A. J., & Mertiny, P. (2020). Development and characterization of stable polymer formulations for manufacturing magnetic composites. *Journal of Manufacturing and Materials Processing, 4*(1), 4.

Nandy, A., Radović, J. R., Novotnik, B., Sharma, M., Larter, S. R., & Thangadurai, V. (2020). Investigation of crude oil degradation using a microbial fuel cell using metal oxide based anode. *Bioresource Technology Reports,* 100449.

Novotnik, B., Nandy, A., Venkatesan, S. V., Radović, J. R., De La Fuente, J., Nejadi, S., Silva, R. C., Kouris, A., Thangadurai, V., Bryant, S., Karan, K., Shor, R., Strous, M. & Larter, S. (2020). Can fossil fuel energy be recovered and used without any CO_2 emissions to the atmosphere? *Reviews in Environmental Science and Bio/Technology,* 1-24.

Pan, W., Innanen, K. A., & Wang, Y. (2020). Parameterization analysis and field validation of VTI-elastic full-waveform inversion in a walk-away vertical seismic profile configuration. *Geophysics, 85*(3), B87-B107.

Park, S., Siahrostami, S., Park, J., Mostaghimi, A. H. B., Kim, T. R., Vallez, L., Gill, T. M., Park, W., Goodson, K. E., Sinclair, R., & Zheng, X. (2020). Effect of Adventitious Carbon on Pit Formation of Monolayer MoS2. *Advanced Materials,* 2003020.

Pinto, H., Gates, I., & Wang, X. (2020). Bayesian biclustering by dynamics: Algorithm testing, comparison against random agglomeration, and calculation of application specific prior information. *MethodsX,* 100897.

Prathapan, R., Tabor, R. F., Garnier, G., & Hu, J. (2020). Recent progress in cellulose nanocrystal alignment and its applications. *ACS Applied Bio Materials, 3*(4), 1828-1844.

Rahman, M. Z., Kibria, M. G., & Mullins, C. B. (2020). Metal-free photocatalysts for hydrogen evolution. *Chemical Society Reviews, 49*(6), 1887-1931.

Rodríguez-Pradilla, G., & Eaton, D. W. (2020). Ground-motion analysis of hydraulic-fracturing induced seismicity at close epicentral distance. *Bulletin of the Seismological Society of America, 110*(1), 331-344.

Shabib-Asl, A., Plaksina, T., & Moradi, B. (2020). Evaluation of nanopore confinement during CO_2 huff and puff process in liquid-rich shale formations. *Computational Geosciences,* 1-16.

Sharma, M., Nandy, A., Taylor, N., Venkatesan, S. V., Kollath, V. O., Karan, K., Thangadurai, V., Tsesmetzis, N., & Gieg, L. M. (2020). Bioelectrochemical remediation of phenanthrene in a microbial fuel cell using an anaerobic consortium enriched from a hydrocarbon-contaminated site. *Journal of Hazardous Materials,* 389, 121845.

Shrivastava, U. N., Suetsugu, K., Nagano, S., Fritzsche, H., Nagao, Y., & Karan, K. (2020). Cross-correlated humidity-dependent structural evolution of Nafion thin films confined on a platinum substrate. *Soft Matter, 16*(5), 1190-1200.

Siahrostami, S., Jimenez Villegas, S., Bagherzadeh Mostaghimi, A. H., Back, S., Barati Farimani, A., Wang, H., Persson, K. A., & Montoya, J. H. (2020). A review on challenges and successes in atomic scale design of catalysts for electrochemical synthesis of hydrogen peroxide. *ACS Catalysis.*

Silva, R. C., Yim, C., Radović, J. R., Brown, M., Weerawardhena, P., Huang, H., Snowden, L. R., Oldenburg, T. B. P., & Larter, S. R. (2020). Mechanistic insights into sulfur rich oil formation, relevant to geological carbon storage routes. A study using (+) APPI FTICR-MS analysis. *Organic Geochemistry,* 104067.

Song, P., & Lu, Q. (2020). Porous clusters of metal-organic framework coated stainless steel mesh for highly efficient oil/water separation. *Separation and Purification Technology,* 238, 116454.

Song, P., Mao, X., Ren, Y., Zeng, H., & Lu, Q. (2020). Buckling effect of sole Zeolitic Imidazolate Framework-8 nanoparticles adsorbed at the water/oil interface. *Langmuir, 36*(9), 2322-2329.

Tawiah, P., Duer, J., Bryant, S. L., Larter, S., O'Brien, S., & Dong, M. (2020). CO_2 injectivity behaviour under non-isothermal conditions–field observations and assessments from the Quest CCS operation. *International Journal of Greenhouse Gas Control, 92*, 102843.

Tian, D., Zhong, N., Leung, J., Shen, F., Hu, J., & Saddler, J. N. (2020). Potential of xylanases to reduce the viscosity of micro/nanofibrillated bleached kraft pulp. *ACS Applied Bio Materials, 3*(4), 2201-2208.

Venkatesan, S. V., Karan, K., Larter, S. R., & Thangadurai, V. (2020). An auxiliary electrode mediated membrane-free redox electrochemical cell for energy storage. *Sustainable Energy & Fuels, 4*(5), 2149-2152.

Wang, J., Xie, L., Lu, Q., Wang, X., Wang, J., & Zeng, H. (2020). Electrochemical investigation of the interactions of organic and inorganic depressants on basal and edge planes of molybdenite. *Journal of Colloid and Interface Science.*

Wang, Q., Huang, H., Chen, H., & Zhao, Y. (2020). Secondary alteration of ancient Shuntuoguole oil reservoirs, Tarim Basin, NW China. *Marine and Petroleum Geology, 111,* 202-218.

Wang, Y., & Lu, Q. (2020). Dendrimer functionalized nanocrystalline cellulose for Cu (II) removal. *Cellulose, 27*(4), 2173-2187.

Wang, Z., Wu, Y., Wu, C., Xie, J., Gu, X., Yu, P., Zong, M., Gates, I. D., Liu, H., & Rong, J. (2020). Electrophilic oxygen on defect-rich carbon nanotubes for selective oxidation of cyclohexane. *Catalysis Science & Technology, 10*(2), 332-336.

Wei, W., Wang, J., Afshordi, S., & Gates, I. D. (2020). Detailed analysis of Toe-to-Heel Air Injection for heavy oil production. *Journal of Petroleum Science and Engineering, 186,* 106704.

Xia, C., Back, S., Ringe, S., Jiang, K., Chen, F., Sun, X., Siahrostami, S., Chan, K., & Wang, H. (2020). Confined local oxygen gas promotes electrochemical water oxidation to hydrogen peroxide. *Nature Catalysis, 3*(2), 125-134.

Xiao, Y., & Hill, J. M. (2020). Solid acid catalysts produced by sulfonation of petroleum coke: Dominant role of aromatic hydrogen. *Chemosphere, 248,* 125981.

Yang, W., Xu, S., Ma, K., Wu, C., Gates, I. D., Ding, X., Meng, W., & Gao, Z. (2020). Geometric structures, electronic characteristics, stabilities, catalytic activities, and descriptors of graphene-based single-atom catalysts. *Nano Materials Science, 2*(2), 120-131.

Yang, W., Huang, H., Ding, X., Ding, Z., Wu, C., Gates, I. D., & Gao, Z. (2020). Theoretical study on double-atom catalysts supported with graphene for electroreduction of nitrogen into ammonia. *Electrochimica Acta, 335,* 135667.

Yang, W., Li, L., Zhao, M., Huang, H., Ding, X., Wu, C., Gates, I. D., & Gao, Z. (2020). Theoretical prediction of graphene-based single-atom iron as a novel catalyst for catalytic oxidation of Hg0 by O_2. *Applied Surface Science, 508,* 145035.

Yang, W., Zhao, M., Ding, X., Ma, K., Wu, C., Gates, I. D., & Gao, Z. (2020). The effect of coordination environment on the kinetic and thermodynamic stability of single-atom iron catalysts. *Physical Chemistry Chemical Physics, 22*(7), 3983-3989.

Yang, W., Xu, S., Ma, K., Wu, C., Gates, I. D., Ding, X., Meng, W., & Gao, Z. (2020). Geometric structures, electronic characteristics, stabilities, catalytic activities, and descriptors of graphene-based single-atom catalysts. *Nano Materials Science, 2*(2), 120-131.

Yin, M., Huang, H., Brown, M., Lucach, S. O., Caminero, L. G., Chavez, S. M., & Oldenburg, T. B. (2020). A novel biodegradation parameter derived from bicyclic sesquiterpanes for assessing moderate levels of petroleum biodegradation. *Organic Geochemistry,* 104049.

Yu, X., Li, J., Chen, Z., Wu, K., Zhang, L., & Yang, S. (2020). Effects of helium adsorption in carbon nanopores on apparent void volumes and excess methane adsorption isotherms. *Fuel, 270,* 117499.

Yu, X., Li, J., Chen, Z., Wu, K., & Zhang, L. (2020). Effects of an adsorbent accessible volume on methane adsorption on shale. *Computer Methods in Applied Mechanics and Engineering, 370*, 113222.

Yu, X., Li, J., Chen, Z., Wu, K., Zhang, L., Hui, G., & Yang, M. (2020). Molecular dynamics computations of brine-CO_2/CH_4-shale contact angles: Implications for CO_2 sequestration and enhanced gas recovery. Fuel, 280, 118590.

Zargartalebi, M., Benneker, A. M., & Azaiez, J. (2020). The impact of heterogeneous pin based micro-structures on flow dynamics and heat transfer in micro-scale heat exchangers. *Physics of Fluids, 32*(5), 052007.

Zecevic, M., Eyre, T. S., & Eaton, D. W. (2020). Static ground displacement for an induced earthquake recorded on broadband seismometers. Bulletin of the Seismological Society of America.

Zhai, R., Hu, J., Chen, X., Xu, Z., Wen, Z., & Jin, M. (2020). Facile synthesis of manganese oxide modified lignin nanocomposites from lignocellulosic biorefinery wastes for dye removal. *Bioresource Technology,* 123846.

Zhang, H., Huang, H., Li, Z., & Liu, M. (2020). Comparative study between sequential solvent-extraction and multiple isothermal stages pyrolysis: A case study on Eocene Shahejie Formation shales, Dongying Depression, East China. *Fuel, 263,* 116591.

Zhang, Y., Khorshidian, H., Ashani, M. M., Sanati-Nezhad, A., & Hejazi, S. H. (2020). Functionalized multiscale visual models to unravel flow and transport physics in porous structures. *Water Research,* 115676.

Zhang, Z., Singh, K., Tsur, Y., Zhou, J., Dynes, J., & Thangadurai, V. (2020). Studies on effect of Ca-doping on structure and electrochemical properties of garnet-type $Y_{3-x}Ca_xFe_5O_{12-\delta}$. *Journal of Solid State Chemistry,* 121530.

Aarsnes, U. J. F., Auriol, J., Di Meglio, F., & Shor, R. J. (2019). Estimating friction factors while drilling. *Journal of Petroleum Science and Engineering, 179,* 80-91.

Abd-Ellah, M., Cann, J., Dayneko, S. V., Laventure, A., Cieplechowicz, E., & Welch, G. C. (2019). Interfacial ZnO modification using a carboxylic acid functionalized N-annulated perylene diimide for inverted type organic photovoltaics. *ACS Applied Electronic Materials, 1*(8), 1590-1596.

Ataeian, M., Liu, Y., Canon-Rubio, K. A., Nightingale, M., Strous, M., & Vadlamani, A. (2019). Direct capture and conversion of CO_2 from air by growing a cyanobacterial consortium at pH up to 11.2. *Biotechnology and bioengineering, 116*(7), 1604-1611.

Auriol, J., Kazemi, N., Shor, R. J., Innanen, K. A., & Gates, I. D. (2019). A sensing and computational framework for estimating the seismic velocities of rocks interacting with the drill bit. *IEEE Transactions on Geoscience and Remote Sensing, 58*(5), 3178-3189.

Austin-Adigio, M., & Gates, I. (2019). Cleaner production from Steam-Assisted Gravity Drainage using seismic-based automated control. *Journal of Cleaner Production, 209,* 1139-1151.

Austin-Adigio, M., & Gates, I. (2019). Non-condensable gas co-injection with steam for oil sands recovery. *Energy, 179,* 736-746.

Badran, I., A.D. Manasrah, and N. N. Nassar, (2019) A Combined Experimental and Density Functional Theory Study of Metformin Oxy-Cracking for Pharmaceutical Wastewater Treatment, *RSC Advance, 9(*24), 13403-13413

Banerjee, A., Bertolesi, G. E., Ling, C. C., Blasiak, B., Purchase, A., Calderon, O., Tomanek, B., & Trudel, S. (2019). Bifunctional pyrrolidin-2-one terminated manganese oxide nanoparticles for combined magnetic resonance and fluorescence imaging. *ACS Applied Materials & Interfaces, 11*(14), 13069-13078.

Bazazi, P., Sanati-Nezhad, A., & Hejazi, S. H. (2019). Wetting phase disintegration and detachment: Three-dimensional confocal imaging of two-phase distributions. *Physical Review Applied, 11*(1), 014042.

Bazazi, P., Sanati-Nezhad, A., & Hejazi, S. H. (2019). Role of chemical additives on water-based heavy oil mobilization: A microfluidic approach. *Fuel, 241,* 1195-1202.

Cao, C., Singh, K., Kan, W. H., Avdeev, M., & Thangadurai, V. (2019). Electrical properties of hollandite-type $Ba_{1.33}Ga_{2.67}Ti_{5.33}O_{16}$, $K_{1.33}Ga_{1.33}Ti_{6.67}O_{16}$, and $K_{1.54}Mg_{0.77}Ti_{7.23}O_{16}$. Inorganic Chemistry, 58(8), 4782-4791.

Chen, Z., Lin, M., Wang, S., Chen, S., & Cheng, L. (2019). Impact of un-propped fracture conductivity on produced gas huff-n-puff performance in Montney liquid rich tight reservoirs. *Journal of Petroleum Science and Engineering, 181,* 106234.

Chernyshova, I. V., & Ponnurangam, S. (2019). Activation of CO_2 at the electrode–electrolyte interface by a co-adsorbed cation and an electric field. *Physical Chemistry Chemical Physics, 21*(17), 8797-8807.

Ciszkowski, C., Ouled Ameur, Z., Forsyth, J., Nightingale, M., Shevalier, M., & Mayer, B. (2019). Application of geochemical and isotopic tracers for characterization of SAGD waters in the Alberta oil-sand region. *SPE Production & Operations, 35,* 188-201.

Dong, X., & Strous, M. (2019). An integrated pipeline for annotation and visualization of metagenomic contigs. *Frontiers in Genetics, 10,* 999.

Dubrawski, Z., Heidebrecht, J., Lombardi, B. M. P., Hyla, A. S., Willkomm, J., Radford, C. L., Lin, J-B., Welch, G. C., Ponnurangam, S., Roesler, R., Prokopchuk, D. E., & Piers, W. E. (2019). Ligand-centered electrochemical processes enable CO_2 reduction with a nickel bis (triazapentadienyl) complex. *Sustainable Energy & Fuels, 3*(5), 1172-1181.

Elahi, S. M., Scott, C. E., Chen, Z., & Pereira-Almao, P. (2019). In-situ upgrading and enhanced recovery of heavy oil from carbonate reservoirs using nano-catalysts: Upgrading reactions analysis. *Fuel, 252,* 262-271.

Esmaeili, S., Sarma, H., Harding, T., & Maini, B. (2019). A data-driven model for predicting the effect of temperature on oil-water relative permeability. *Fuel, 236,* 264-277.

Esmaeili, S., Sarma, H., Harding, T., & Maini, B. (2019). Correlations for effect of temperature on oil/water relative permeability in clastic reservoirs. *Fuel, 246,* 93-103.

Esmaeili, S., Sarma, H., Harding, T., & Maini, B. (2019). Review of the effect of temperature on oil-water relative permeability in porous rocks of oil reservoirs. *Fuel, 237,* 91-116.

Eyre, T. S., Eaton, D. W., Garagash, D. I., Zecevic, M., Venieri, M., Weir, R., & Lawton, D. C. (2019). The role of aseismic slip in hydraulic fracturing–induced seismicity. *Science Advances, 5*(8), eaav7172.

Eyre, T. S., Eaton, D. W., Zecevic, M., D'Amico, D., & Kolos, D. (2019). Microseismicity reveals fault activation before Mw 4.1 hydraulic-fracturing induced earthquake. *Geophysical Journal International, 218*(1), 534-546.

Gendy, C., Mansikkamäki, A., Valjus, J., Heidebrecht, J., Hui, P. C. Y., Bernard, G. M., Tuononen, H. M., Wasylishen, R. E., Michaelis, V. K., & Roesler, R. (2019). Nickel as a Lewis base in a T-shaped Nickel (0) Germylene complex incorporating a flexible bis (NHC) ligand. *Angewandte Chemie International Edition, 58*(1), 154-158.

He, C., Huang, H., Wang, Q., & Li, Z. (2019). Correlation of maturity parameters derived from methylphenanthrenes and methyldibenzothiophenes in the carboniferous source rocks from Qaidam Basin, NW China. *Geofluids, 2019,* Article ID 5742902.

Hinzke, T., Kouris, A., Hughes, R. A., Strous, M., & Kleiner, M. (2019). More is not always better: Evaluation of 1D and 2D-LC-MS/MS methods for metaproteomics. *Frontiers in Microbiology, 10,* 238.

Huang, H., Li, Z., Wen, Z., Han, D., & Pan, R. (2019). Biodegradation influence on alkylphenanthrenes in oils from Bongor Basin, SW Chad. *Scientific Reports, 9*(1), 1-11.

Jiang, K., Back, S., Akey, A. J., Xia, C., Hu, Y., Liang, W., Schaak, D., Stavitski, E., Nørskov, J. K., Siahrostami, S., & Wang, H. (2019). Highly selective oxygen reduction to hydrogen peroxide on transition metal single atom coordination. *Nature Communications, 10*(1), 1-11.

Jin, Z., Zhou, M., Hu, J., Li, K., Tang, L., Zhao, H., Cai, Z., & Zhao, Y. (2019). Hierarchical Ni@ Ni $(OH)_2$ core-shell hybrid arrays on cotton cloth fabricated by a top-down approach for high-performance flexible asymmetric supercapacitors. *Journal of Alloys and Compounds, 784*, 1091-1098.

Kazemi, N., Trad, D., Innanen, K., & Shor, R. (2019). Least-squares RTM of a seismic-while-drilling dataset. *arXiv preprint* arXiv:1902.06889.

Koenig, J. D., Laventure, A., & Welch, G. C. (2019). Harnessing direct (hetero) arylation in pursuit of a saddle-shaped perylene diimide tetramer. *ACS Applied Energy Materials, 2*(12), 8939-8945.

Koenig, J. D., Willkomm, J., Roesler, R., Piers, W. E., & Welch, G. C. (2019). Electrocatalytic CO_2 reduction at lower overpotentials using Iron (III) Tetra (meso-thienyl) porphyrins. *ACS Applied Energy Materials, 2*(6), 4022-4026.

Kreider, M. E., Gallo, A., Back, S., Liu, Y., Siahrostami, S., Nordlund, D., Sinclair, R., Nørskov, J. K., Kng, La A., & Jaramillo, T. F. (2019). Precious metal-free nickel nitride catalyst for the oxygen reduction reaction. *ACS Applied Materials & Interfaces, 11*(30), 26863-26871.

Larter, S., Silva, R. C., Marcano, N., Snowdon, L. R., Villarreal-Barajas, J. E., Sonei, R., Gutierrez, L. C. P., Huang, H., Stopford, A., Oldenburg, T. B. P., Zhao, J., Weewardhena, P., Nightingale, M., Mayer, B., Pedersen J. H., & di Primio, R. (2019). The dating of petroleum fluid residence time in subsurface reservoirs. Part 1: A radiolysis-based geochemical toolbox. *Geochimica et Cosmochimica Acta, 261,* 305-326.

Laventure, A., Stanzel, S., Payne, A. J., Lessard, B. H., & Welch, G. C. (2019). A ring fused N-annulated PDI non-fullerene acceptor for high open circuit voltage solar cells processed from non-halogenated solvents. *Synthetic Metals, 250,* 55-62.

Laventure, A., Harding, C. R., Cieplechowicz, E., Li, Z., Wang, J., Zou, Y., & Welch, G. C. (2019). Screening quinoxaline-type donor polymers for roll-to-roll processing compatible organic photovoltaics. *ACS Applied Polymer Materials, 1*(8), 2168-2176.

Li, J., Innanen, K. A., Wang, B., & Tao, G. (2019). Azimuth ambiguity elimination for borehole imaging using 3D borehole RTM scheme. *Journal of Applied Geophysics, 166,* 103-111.

Li, J., Wu, K., Chen, Z., Wang, K., Luo, J., Xu, J., Li, R., Yu, R., & Li, X. (2019). On the negative excess isotherms for methane adsorption at high pressure: modeling and experiment. *SPE Journal, 24,* 2504-2525.

Li, J., Wu, K., Chen, Z., Wang, W., Yang, B., Wang, K., Luo, J., & Yu, R. (2019). Effects of energetic heterogeneity on gas adsorption and gas storage in geologic shale systems. *Applied Energy, 251,* 113368.

Li, R., Wu, K., Li, J., Xu, J., & Chen, Z. (2019). Shale gas transport in wedged nanopores with water films. *Journal of Natural Gas Science and Engineering, 66,* 217-232.

Li, Z., Huang, H., He, C., & Fang, X. (2019). Maturation impact on polyaromatic hydrocarbons and organosulfur compounds in the Carboniferous Keluke Formation from Qaidam Basin, NW China. *Energy & Fuels, 33*(5), 4115-4129.

Long, L., Hu, J., Li, X., Zhang, Y., & Wang, F. (2019). The potential of using thermostable xylan-binding domain as a molecular probe to better understand the xylan distribution of cellulosic fibers. *ACS Sustainable Chemistry & Engineering, 7*(14), 12520-12526.

Long, L., Shen, F., Wang, F., Tian, D., & Hu, J. (2019). Synthesis, characterization and enzymatic surface roughing of cellulose/xylan composite films. *Carbohydrate Polymers, 213,* 121-127.

Maan, O., Song, P., Chen, N., & Lu, Q. (2019). An in situ procedure for the preparation of Zeolitic Imidazolate Framework-8 polyacrylamide hydrogel for adsorption of aqueous pollutants. *Advanced Materials Interfaces, 6*(10), 1801895.

Mammoottil Abraham, A., Kammampata, S. P., Ponnurangam, S., & Thangadurai, V. (2019). Efficient synthesis and characterization of robust MoS_2 and S cathode for advanced Li–S battery: Combined experimental and theoretical studies. *ACS Applied Materials & Interfaces, 11*(39), 35729-35737.

Manasrah, A. D, A. Hassan and N. N. Nassar, (2019). Enhancement of Petroleum Coke Thermal Reactivity using Oxy-Cracking Technique. *The Canadian Journal of Chemical Engineering, 97*(11), 2794-2803.

Manjón-Sanz, A., Culbertson, C. M., Hou, D., Jones, J. L., & Dolgos, M. R. (2019). Total scattering and diffraction studies of lead-free piezoelectric (1-x) Ba $(Zr_{0.2}Ti_{0.8})$ O_{3-x} $(Ba_{0.7}Ca_{0.3})$ TiO_3 deconvolute intrinsic and extrinsic contributions to electromechanical strain. *Acta Materialia, 171,* 79-91.

Macquet, M., Lawton, D. C., Saeedfar, A., & Osadetz, K. G. (2019). A feasibility study for detection thresholds of CO_2 at shallow depths at the CaMI Field Research Station, Newell County, Alberta, Canada. *Petroleum Geoscience, 25*(4), 509-518.

McKean, S. H., Priest, J. A., Dettmer, J., & Eaton, D. W. (2019). Quantifying fracture networks inferred from microseismic point clouds by a Gaussian mixture model with physical constraints. *Geophysical Research Letters, 46*(20), 11008-11017.

McKean, S. H., & Priest, J. A. (2019). Multiple failure state triaxial testing of the Montney Formation. *Journal of Petroleum Science and Engineering, 173,* 122-135.

Meng, C., Hu, J., Gourlay, K., Yu, C., & Saddler, J. N. (2019). Controllable synthesis uniform spherical bacterial cellulose and their potential applications. *Cellulose, 26*(15), 8325-8336.

Meng, C., Hu, J., Yu, C., & Sun, F. (2019). Evaluation of the mild Mg (OH) 2-AQ aided alkaline oxidation degumming process of ramie fiber at an industrial scale. *Industrial Crops and Products, 137,* 694-701.

Meng, C., Zhong, N., Hu, J., Yu, C., & Saddler, J. N. (2019). The effects of metal elements on ramie fiber oxidation degumming and the potential of using spherical bacterial cellulose for metal removal. *Journal of Cleaner Production, 206,* 498-507.

Mohammadmoradi, P., & Kantzas, A. (2019). Modelling shale spontaneous water intake using semi-analytical and numerical approaches. T*he Canadian Journal of Chemical Engineering, 97,* 1627-1642.

Moud, A. A., Arjmand, M., Liu, J., Yang, Y., Sanati-Nezhad, A., & Hejazi, S. H. (2019). Cellulose nanocrystal structure in the presence of salts. *Cellulose, 26*(18), 9387-9401.

Mulmi, S., & Thangadurai, V. (2019). A perovskite-type $Nd_{0.75}Sr_{0.25}Co_{0.8}Fe_{0.2}O_{3-\delta}$ cathode for advanced solid oxide fuel cells. *Chemical Communications, 55*(26), 3713-3716.

Nafie, G., A. D. Manasrah, B. Mackay, I. Badran, N. N. Nassar,(2019) Oxy-Cracking Reaction for Enhanced Settling and Dewaterability of Oil Sands Tailings, *Industrial & Engineering Chemistry Research, 58* (12), 4988–4996.

Nandy, A., Sharma, M., Venkatesan, S. V., Taylor, N., Gieg, L., & Thangadurai, V. (2019). Comparative evaluation of coated and non-coated carbon electrodes in a microbial fuel cell for treatment of municipal sludge. *Energies, 12*(6), 1034.

Nazari, M., Cieplechowicz, E., Welsh, T. A., & Welch, G. C. (2019). A direct comparison of monomeric vs. dimeric and non-annulated vs. N-annulated perylene diimide electron acceptors for organic photovoltaics. *New Journal of Chemistry,* 43(13), 5187-5195.

Novotnik, B., Zorz, J., Bryant, S., & Strous, M. (2019). The effect of dissimilatory manganese reduction on lactate fermentation and microbial community assembly. *Frontiers in Microbiology, 10*, 1007.

Pan, B., Jones, F., Huang, Z., Yang, Y., Li, Y., Hejazi, S. H., & Iglauer, S. (2019). Methane (CH_4) wettability of clay-coated quartz at reservoir conditions. *Energy & Fuels, 33*(2), 788-795.

Pan, B., Li, Y., Xie, L., Wang, X., He, Q., Li, Y., Hejazi, S. H., & Iglauer, S. (2019). Role of fluid density on quartz wettability. *Journal of Petroleum Science and Engineering, 172,* 511-516.

Pan, W., & Innanen, K. A. (2019). Amplitude-based misfit functions in viscoelastic full-waveform inversion applied to walk-away vertical seismic profile data. *Geophysics, 84*(5), B335-B351.

Pan, W., Innanen, K. A., Geng, Y., & Li, J. (2019). Interparameter trade-off quantification for isotropic-elastic full-waveform inversion with various model parameterizations. *Geophysics, 84*(2), R185-R206.

Pang, Y., Chen, S., Soliman, M. Y., Morse, S. M., & Hu, X. (2019). Evaluation of matrix swelling behavior in shale induced by methane sorption under triaxial stress and strain conditions. *Energy & Fuels, 33*(6), 4986-5000.

Pang, Y., Chen, S., Soliman, M. Y., Morse, S. M., & Hu, X. (2019). Evaluation of matrix swelling behavior in shale induced by methane sorption under triaxial stress and strain conditions. *Energy & Fuels, 33*(6), 4986-5000.

Pinto, H., Gates, I., & Wang, X. (2019). Bayesian Biclustering by dynamics: A clustering algorithm for SAGD time series data. *Computers & Geosciences, 133,* 104304.

Poulin, A., Weir, R., Eaton, D., Igonin, N., Chen, Y., Lines, L., & Lawton, D. (2019). Focal-time analysis: A new method for stratigraphic depth control of microseismicity and induced seismic events. *Geophysics, 84*(6), KS173-KS182.

Shabib-Asl, A., & Plaksina, T. (2019). Selection of decline curve analysis model using Akaike information criterion for unconventional reservoirs. *Journal of Petroleum Science and Engineering, 182,* 106327.

Silva, R. C., Snowdon, L. R., Huang, H., Nightingale, M., Becker, V., Taylor, S., Mayer, B., Pedersen, J. H., di Primio, R., & Larter, S. (2019). Radiolysis as a source of 13C depleted natural gases in the geosphere. *Organic Geochemistry, 138*, 103911.

Singh, K., Kannan, R., & Thangadurai, V. (2019). Perspective of perovskite-type oxides for proton conducting solid oxide fuel cells. *Solid State Ionics, 339,* 114951.

Song, P., Natale, G., Wang, J., Bond, T., Hejazi, H., Siegler, H. D. L. H., Gates, I., & Lu, Q. (2019). 2D and 3D metal–organic framework at the oil/water interface: A case study of copper benzenedicarboxylate. *Advanced Materials Interfaces, 6*(2), 1801139.

Tarokh, A., Karan, K., & Ponnurangam, S. (2019). Atomistic MD study of nafion dispersions: Role of solvent and counterion in the aggregate structure, ionic clustering, and acid dissociation. *Macromolecules, 53*(1), 288-301.

Tintori, F., Laventure, A., & Welch, G. C. (2019). Additive induced crystallization of a twisted perylene diimide dimer within a polymer matrix. *Soft Matter, 15*(25), 5138-5146.

Tintori, F., Laventure, A., & Welch, G. C. (2019). Perylene diimide based organic photovoltaics with slot-die coated active layers from halogen-free solvents in air at room temperature. *ACS Applied Materials & Interfaces, 11*(42), 39010-39017.

Vishkai, M., & Gates, I. (2019). On multistage hydraulic fracturing in tight gas reservoirs: Montney Formation, Alberta, Canada. *Journal of Petroleum Science and Engineering, 174,* 1127-1141.

Wang, Q., Huang, H., Li, Z., & Li, Z. (2019). Novel thermal maturity parameters derived from alkylbiphenyls and alkyldiphenylmethanes. *Energy & Fuels, 33*(9), 8491-8502.

Weir, R., Lawton, D., Lines, L., Eyre, T., & Eaton, D. (2019). Application of structural interpretation and simultaneous inversion to reservoir characterization of the Duvernay Formation, Fox Creek, Alberta, Canada. *The Leading Edge, 38*(2), 151-160.

Welsh, T. A., Laventure, A., Alahmadi, A. F., Zhang, G., Baumgartner, T., Zou, Y., Jakle, F., & Welch, G. C. (2019). Borane incorporation in a non-fullerene acceptor to tune steric and electronic properties and improve organic solar cell performance. *ACS Applied Energy Materials, 2*(2), 1229-1240.

Willkomm, J., Bertin, E., Atwa, M., Lin, J. B., Birss, V., & Piers, W. E. (2019). Grafting of a molecular rhenium CO_2 reduction catalyst onto colloid-imprinted carbon. *ACS Applied Energy Materials, 2*(4), 2414-2418.

Wu, C., & Gates, I. D. (2019). Methane activation by a single iron atom supported on graphene: Impact of substrates. *Molecular Catalysis, 469,* 40-47.

Wu, C., De Visscher, A., & Gates, I. D. (2019). On naphthenic acids removal from crude oil and oil sands process-affected water. *Fuel, 253,* 1229-1246.

Wu, K., Chen, Z., Li, J., Lei, Z., Xu, J., Wang, K., Li, R., Dong, X., Peng, Y., Yang, S., Zhang, F., Chen, Z. & Gao, Y. (2019). Nanoconfinement effect on n-alkane flow. *The Journal of Physical Chemistry C, 123*(26), 16456-16461.

Wu, K., Chen, Z., Li, J., Xu, J., Wang, K., Li, R., Wang, S., & Dong, X. (2019). Ultrahigh water flow enhancement by optimizing nanopore chemistry and geometry. *Langmuir, 35*(26), 8867-8873.

Xu, X., Huang, H., Zhang, S., & Hu, S. (2019). Gas generation potential and processes of Athabasca oil sand bitumen from gold tube pyrolysis experiments. *Fuel, 239,* 804-813.

Zhai, R., Chen, X., Jin, M., & Hu, J. (2019). Synthesis of a polydopamaine nanoparticle/bacterial cellulose composite for use as a biocompatible matrix for laccase immobilization. *Cellulose, 26*(15), 8337-8349.

Zhang, H., Huang, H., Li, Z., & Liu, M. (2019). Oil physical status in lacustrine shale reservoirs–A case study on Eocene Shahejie Formation shales, Dongying Depression, East China. *Fuel, 257,* 116027.

Zorz, J. K., Sharp, C., Kleiner, M., Gordon, P. M., Pon, R. T., Dong, X., & Strous, M. (2019). A shared core microbiome in soda lakes separated by large distances. *Nature Communications, 10*(1), 1-10.

Amiri, T., Singh, K., Sandhu, N. K., Hanifi, A. R., Etsell, T. H., Luo, J. L., Thangadurai, V., & Sarkar, P. (2018). High performance tubular solid oxide fuel cell based on $Ba_{0.5}Sr_{0.5}Ce_{0.6}Zr_{0.2}Gd_{0.1}Y_{0.1}O_{3-\delta}$ proton conducting electrolyte. *Journal of The Electrochemical Society, 165*(10), F764.

Bazazi, P., Sanati-Nezhad, A., & Hejazi, S. H. (2018). Wetting dynamics in two-liquid systems: Effect of the surrounding phase viscosity. *Physical Review E, 97*(6), 063104.

Chen, H., & Innanen, K. A. (2018). Estimation of fracture weaknesses and integrated attenuation factors from azimuthal variations in seismic amplitudes. *Geophysics, 83*(6), R711-R723.

Chen, H., Innanen, K. A., & Chen, T. (2018). Estimating P-and S-wave inverse quality factors from observed seismic data using an attenuative elastic impedance. *Geophysics, 83*(2), R173-R187.

Chen, H., Ji, Y., & Innanen, K. A. (2018). Estimation of modified fluid factor and dry fracture weaknesses using azimuthal elastic impedance. *Geophysics, 83*(1), WA73-WA88.

Chen, Q., Liu, D., Wu, C., Yao, K., Li, Z., Shi, N., wen, F., & Gates, I. D. (2018). Co-immobilization of cellulase and lysozyme on amino-functionalized magnetic nanoparticles: An activity-tunable biocatalyst for extraction of lipids from microalgae. *Bioresource Technology, 263,* 317-324.

Chernyshova, I. V., Somasundaran, P., & Ponnurangam, S. (2018). On the origin of the elusive first intermediate of CO_2 electroreduction. *Proceedings of the National Academy of Sciences, 115*(40), E9261-E9270.

Dayneko, S. V., Hendsbee, A. D., & Welch, G. C. (2018). Combining facile synthetic methods with greener processing for efficient polymer-perylene diimide based organic solar cells. *Small Methods, 2*(6), 1800081.

Dayneko, S. V., Payne, A. J., & Welch, G. C. (2018). Inverted P3HT: PC61BM organic solar cells incorporating a ϖ-extended squaraine dye with H-and (or) J-aggregation. *Canadian Journal of Chemistry, 96*(7), 703-711.

Forde, O. N., Mayer, K. U., Cahill, A. G., Mayer, B., Cherry, J. A., & Parker, B. L. (2018). Vadose zone gas migration and surface effluxes after a controlled natural gas release into an unconfined shallow aquifer. *Vadose Zone Journal, 17*(1), 1-16.

Geng, Y., Pan, W., & Innanen, K. A. (2018). Frequency-domain full-waveform inversion with non-linear descent directions. *Geophysical Journal International, 213*(2), 739-756.

Guo, T., Wang, J., & Gates, I. D. (2018). Pad-scale control improves SAGD performance. *Petroleum, 4*(3), 318-328.

Jia, S. Q., Eaton, D. W., & Wong, R. C. (2018). Stress inversion of shear-tensile focal mechanisms with application to hydraulic fracture monitoring. *Geophysical Journal International, 215*(1), 546-563.

Kannaiyan, R., Wang, J., & Gates, I. D. (2018). Microemulsion phase formation at oil–cellulose microcrystal suspension interfaces. *Cellulose, 25*(3), 1625-1636.

Kleiner, M., Dong, X., Hinzke, T., Wippler, J., Thorson, E., Mayer, B., & Strous, M. (2018). Metaproteomics method to determine carbon sources and assimilation pathways of species in microbial communities. *Proceedings of the National Academy of Sciences, 115*(24), E5576-E5584.

Lal, G., Derakhshandeh, M., Akhtar, F., Spasyuk, D. M., Lin, J. B., Trifkovic, M., & Shimizu, G. K. (2018). Mechanical properties of a metal–organic framework formed by covalent cross-linking of metal–organic polyhedra. *Journal of the American Chemical Society, 141*(2), 1045-1053.

Laventure, A., & Welch, G. C. (2018). A tetrachlorinated molecular non-fullerene acceptor for high performance near-IR absorbing organic solar cells. *Journal of Materials Chemistry C, 6*(34), 9060-9064.

Li, J., Chen, Z., Wu, K., Wang, K., Luo, J., Feng, D., Qu, S., & Li, X. (2018). A multi-site model to determine supercritical methane adsorption in energetically heterogeneous shales. *Chemical Engineering Journal, 349,* 438-455.

Li, J., Chen, Z., Wu, K., Zhang, T., Zhang, R., Xu, J., Li, R., Qu, S., Shi, J., & Li, X. (2018). Effect of water saturation on gas slippage in circular and angular pores. *AIChE Journal, 64*(9), 3529-3541.

Li, T., Sharp, C. E., Ataeian, M., Strous, M., & De Beer, D. (2018). Role of extracellular carbonic anhydrase in dissolved inorganic carbon uptake in alkaliphilic phototrophic biofilm. *Frontiers in Microbiology, 9,* 2490.

Cruz Luque, M. M., Urban-Rascon, E., Aguilera, R. F., & Aguilera, R. (2018). Mexican Unconventional Plays: Geoscience, Endowment, and Economic Considerations. *SPE Reservoir Evaluation & Engineering, 21*(03), 533-549.

Lussier, J. A., Simon, F. J., Whitfield, P. S., Singh, K., Thangadurai, V., & Bieringer, M. (2018). Structure Evolution and Reactivity of the Sc (2–x) V x O3+ δ (0≤ x≤ 2.0) System. *Inorganic Chemistry, 57*(9), 5607-5614.

Maan, O., Huang, J., Zeng, H., & Lu, Q. (2018). Probing molecular interactions between humic acid and surface-grafted polyacrylamide using quartz crystal microbalance with dissipation and atomic force microscopy: implications for environmental remediation. *Environmental Chemistry, 15*(6), 336-350.

Manasrah, D. A., N. N. Nassar, L. C. Ortega (2018). Conversion of petroleum coke into valuable products using oxy-cracking technique. *Fuel, 215,* 865-878

Manjón-Sanz, A. M., & Dolgos, M. R. (2018). Applications of piezoelectrics: old and new. *Chemistry of Materials, 30*(24), 8718-8726.

Mcintosh, J. C., Hendry, M. J., Ballentine, C., Haszeldine, R. S., Mayer, B., Etiope, G., Elsner, M., Darrah, T. H., Prinzhofer, A., Stalker, L., Kuloyo, O., Lu, Z-T., Martini, A., & Sherwood Lollar, B. (2018). A critical review of state-of-the-art and emerging approaches to identify fracking-derived gases and associated contaminants in aquifers. *Environmental Science & Technology, 53*(3), 1063-1077.

Mohammadmoradi, P., Taheri, S., Bryant, S. L., & Kantzas, A. (2018). Solvent diffusion and dispersion in partially saturated porous media: An experimental and numerical pore-level study. *Chemical Engineering Science, 191,* 300-317.

Moud, A. A., Arjmand, M., Yan, N., Nezhad, A. S., & Hejazi, S. H. (2018). Colloidal behavior of cellulose nanocrystals in presence of sodium chloride. *ChemistrySelect, 3*(17), 4969-4978.

Nazari, M., Martell, M., Welsh, T. A., Melville, O., Li, Z., Cann, J., Cieplechowicz, E., Zou, Y., Lessard, B. H., & Welch, G. C. (2018). Benzyl and fluorinated benzyl side chains for perylene diimide non-fullerene acceptors. *Materials Chemistry Frontiers, 2*(12), 2272-2276.

Osadetz, K. G., Mort, A., Snowdon, L. R., Lawton, D. C., Chen, Z., & Saeedfar, A. (2018). Western Canada Sedimentary Basin petroleum systems: A working and evolving paradigm. *Interpretation, 6*(2), SE63-SE98.

Osselin, F., Nightingale, M., Hearn, G., Kloppmann, W., Gaucher, E., Clarkson, C. R., & Mayer, B. (2018). Quantifying the extent of flowback of hydraulic fracturing fluids using chemical and isotopic tracer approaches. *Applied Geochemistry, 93,* 20-29.

Oz, A., Singh, K., Gelman, D., Thangadurai, V., & Tsur, Y. (2018). Understanding of oxygen reduction reaction on perovskite-type $Ba_{0.5}Sr_{0.5}Fe_{0.91}Al_{0.09}O_{3-\delta}$ and $Ba_{0.5}Sr_{0.5}Fe_{0.8}Cu_{0.2}O_{3-\delta}$ using AC impedance spectroscopy genetic programming. *The Journal of Physical Chemistry C, 122*(27), 15097-15107.

Pan, W., Geng, Y., & Innanen, K. A. (2018). Interparameter trade-off quantification and reduction in isotropic-elastic full-waveform inversion: Synthetic experiments and Hussar land data set application. *Geophysical Journal International, 213*(2), 1305-1333.

Pan, W., Innanen, K. A., & Geng, Y. (2018). Elastic full-waveform inversion and parametrization analysis applied to walk-away vertical seismic profile data for unconventional (heavy oil) reservoir characterization. *Geophysical Journal International, 213*(3), 1934-1968.

Pedersen, P. K., & Eaton, D. W. (2018). Introduction to special section: Low-permeability resource plays of the Western Canada Sedimentary Basin—Defining the sweet spots. *Interpretation, 6* (2): SEi–SEii.

Siahrostami, S. (2018). Designing carbon-based materials for efficient electrochemical reduction of CO_2. *Industrial & Engineering Chemistry Research, 58*(2), 879-885.

Shrivastava, U. N., Fritzsche, H., & Karan, K. (2018). Interfacial and bulk water in ultrathin films of Nafion, 3M PFSA, and 3M PFIA ionomers on a polycrystalline platinum surface. *Macromolecules, 51*(23), 9839-9849.

Singh, K., Kan, W. H., Patton, B., Huq, A., & Thangadurai, V. (2018). Insights into B-site ordering in double perovskite-type $Ba_2Ca_{1+x}Nb_{2-x}O_{9-\delta}$ (0≤ x≤ 0.45): Combined synchrotron and neutron diffraction and electrical transport analyses. *Inorganic Chemistry, 57*(5), 2609-2619.

Strous, M., & Sharp, C. (2018). Designer microbiomes forenvironmental, energy and health biotechnology. *Current Opinion in Microbiology, 43,* 117-123.

Welsh, T. A., Laventure, A., & Welch, G. C. (2018). Direct (Hetero) arylation for the synthesis of molecular materials: coupling Thieno [3, 4-c] pyrrole-4, 6-dione with Perylene Diimide to yield novel non-fullerene acceptors for organic solar cells. *Molecules, 23*(4), 931.

Welsh, T. A., Laventure, A., Baumgartner, T., & Welch, G. C. (2018). Dithienophosphole-based molecular electron acceptors constructed using direct (hetero) arylation cross-coupling methods. *Journal of Materials Chemistry C, 6*(8), 2148-2154.

Wu, C., De Visscher, A., & Gates, I. D. (2018). Comparison of electronic and physicochemical properties between imidazolium-based and pyridinium-based ionic liquids. *The Journal of Physical Chemistry B, 122*(26), 6771-6780.

Wu, C., Lü, R., & Gates, I. D. (2018). Computational study on the absorption mechanisms of SO_2 by ionic liquids. *ChemistrySelect, 3*(16), 4330-4338.

Yang, Y., Liu, Z., Yao, J., Zhang, L., Ma, J., Hejazi, S. H., Luquot, L. & Ngarta, T. D. (2018). Flow simulation of artificially induced microfractures using digital rock and lattice Boltzmann methods. *Energies, 11*(8), 2145.

Zorz, J. K., Kozlowski, J. A., Stein, L. Y., Strous, M., & Kleiner, M. (2018). Comparative proteomics of three species of ammonia-oxidizing bacteria. *Frontiers in Microbiology, 9,* 938.

Abdel-Basset, D. M., Mulmi, S., El-Bana, M. S., Fouad, S. S., & Thangadurai, V. (2017). Structure, ionic conductivity, and dielectric properties of Li-rich garnet-type $Li_{5+2x}La_3Ta_{2-x}Sm_xO_{12}$ (0≤ x≤ 0.55) and their chemical stability. *Inorganic Chemistry, 56*(15), 8865-8877.

Basset, D. M. A., Mulmi, S., El-Bana, M. S., Fouad, S. S., & Thangadurai, V. (2017). Synthesis and characterization of novel Li-stuffed garnet-like $Li_{5+2x}La_3Ta_{2-x}Gd_xO1_2$ (0≤ x≤ 0.55): Structure–property relationships. *Dalton Transactions, 46*(3), 933-946.

Cahill, A. G., Steelman, C. M., Forde, O., Kuloyo, O., Ruff, S. E., Mayer, B., Mayer, K. U., Strous, M., Ryan, M. C., Cherry, J. A., & Parker, B. L. (2017). Mobility and persistence of methane in groundwater in a controlled-release field experiment. *Nature Geoscience, 10*(4), 289-294.

Dong, X., Kleiner, M., Sharp, C. E., Thorson, E., Li, C., Liu, D., & Strous, M. (2017). Fast and simple analysis of MiSeq amplicon sequencing data with MetaAmp. *Frontiers in Microbiology, 8,* 1461.

Forshomi, Z. D., Carreon, C. E., Alva-Argaez, A., & Bergerson, J. A. (2017). Energy, water, cost, and greenhouse gas implications of steam-assisted gravity drainage surface facility technologies. *Process Integration and Optimization for Sustainability, 1*(2), 87-107.

Kleiner, M., Thorson, E., Sharp, C. E., Dong, X., Liu, D., Li, C., & Strous, M. (2017). Assessing species biomass contributions in microbial communities via metaproteomics. *Nature communications, 8*(1), 1-14.

Manasrah, D. A., A. El-Qanni, I. Badran, L. C. Ortega, M. J. Perez-Zurita, N. N. Nassar, (2017). Experimental and theoretical studies on oxy-cracking of Quinolin-65 as a model molecule for residual feedstocks. *Reaction Chemistry & Engineering 2*(5), 703-719.

Mulmi, S., Chen, H., Hassan, A., Marco, J. F., Berry, F. J., Sharif, F., Slater, P. R., Roberts, E. P. L., Adams, S., & Thangadurai, V. (2017). Thermochemical CO_2 splitting using double perovskite-type $Ba_2Ca_{0.66}Nb_{1.34-x}Fe_xO_{6-\delta}$. *Journal of Materials Chemistry A, 5*(15), 6874-6883.

Sharp, C. E., Urschel, S., Dong, X., Brady, A. L., Slater, G. F., & Strous, M. (2017). Robust, high-productivity phototrophic carbon capture at high pH and alkalinity using natural microbial communities. *Biotechnology for Biofuels, 10*(1), 1-13.

Conference proceedings/publications

Al-Attas, T. A., & Kibria, M. G. (2020, May). Electrochemical CH_4 oxidation on spinel $NiCo_2O_4$-based composite catalysts. In *237th ECS Meeting with the 18th International Meeting on Chemical Sensors (IMCS 2020)*. ECS.

Auriol, J., Aarsnes, U. J. F., & Shor, R. (2020, July). Self-tuning torsional drilling model for real-time applications. In *2020 American Control Conference (ACC) (pp. 3091-3096).* IEEE.

Auriol, J., Kazemi, N., Innanen, K., & Shor, R. J. (2020, July). Combining formation seismic velocities while drilling and a PDE-ODE observer to improve the drill-string dynamics estimation. In *2020 American Control Conference (ACC) (pp. 3120-3125).* IEEE.

Chen, H., & Innanen, K. (2020, December). Azimuthal Seismic Difference Inversion for Tilted Fracture Weaknesses. In *82nd EAGE Annual Conference & Exhibition (Vol. 2020, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Iverson, A., Keating, S., & Innanen, K. (2020, December). Adaptive subtraction of internal multiple predictions in the downward generator space. In *82nd EAGE Annual Conference & Exhibition Workshop Programme (Vol. 2020, No. 1, pp. 1-3).* European Association of Geoscientists & Engineers.

Kazemi, N., Auriol, J., Innanen, K., Shor, R., & Gates, I. (2020, December). Successive full-waveform inversion of surface seismic and seismic-while-drilling datasets without low frequencies. *In 82nd EAGE Annual Conference & Exhibition (Vol. 2020, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Nejadi, S., Kazemi, N., Curkan, J., Auriol, J., Durkin, P., Hubbard, S., Innanen, K., Shor, R. J., & Gates, I. (2020, March). Look ahead of the bit while drilling: potential impacts and challenges in the McMurray Formation. In *SPE Canada Heavy Oil Conference.*

Rahmanifard, H., Alimohamadi, H., & Gates, I. (2020, July). Well performance prediction in Montney Formation using machine learning approaches. In *SPE/AAPG/SEG Unconventional Resources Technology Conference.* Unconventional Resources Technology Conference.

Salvage, R. O., & Eaton, D. W. (2020, May). Hydraulic fracturing operations within an extremely complex stress regime: The case of Fort St. John, British Columbia, Canada. In *EGU General Assembly Conference Abstracts (p. 5702).*

Abubaker, O. A., Singh, K., & Thangadurai, V. (2019, September). The effect of oxygen partial pressure and composition on the oxygen reduction reaction properties of $Ba_{0.5}Sr_{0.5}Fe_{1-X}Cu_xO_{3-\delta}$ as a cathode for solid oxide fuel cells. In *Meeting Abstracts (No. 40, pp. 1856-1856).* The Electrochemical Society.

Algeer, R., Huang, H., & Larter, S. (2019, September). Constraining the oil charge history of a heavy oilfield using a novel maturity assessment approach: Mass fraction maturity. In *29th International Meeting on Organic Geochemistry (Vol. 2019, No. 1, pp. 1-2).* European Association of Geoscientists & Engineers.

Auriol, J., & Bribiesca-Argomedo, F. (2019, December) Delay-robust stabilization of an n+m hyperbolic PDE-ODE system. In *2019 IEEE 58th Conference on Decision and Control (CDC) (pp. 4964-4970).* IEEE.

Auriol, J., Di Meglio, F., & Bribiesca-Argomedo, F. (2019, July). Delay robust state feedback stabilization of an underactuated network of two interconnected PDE systems. In *2019 American Control Conference (ACC) (pp. 593-599).* IEEE.

Auriol, J., Kazemi, N., Shor, R. J., Innanen, K. A., & Gates, I. D. (2019). a sensing and computational framework for estimating the seismic velocities of rocks interacting with the drill bit. *IEEE Transactions on Geoscience and Remote Sensing, 58*(5), 3178-3189.

Caceres-Falla, M., & De la Hoz Siegler, H. (2019, November) Integrating direct air carbon capture and algal-based bioenergy production. In *2019 AIChE Annual Meeting.* AIChE.

Caceres-Falla, M., & De la Hoz Siegler, H. (2019, November). Modeling chemical absorption of CO_2 in highly alkaline solutions for direct air carbon capture applications. In *2019 AIChE Annual Meeting.* AIChE.

Cahill, A. G., Beckie, R. D., Mayer, B., & Kang, M. (2019, December). Advancing knowledge on subsurface fugitive gas migration from geoenergy development activities through the critical zone: Fundamental science, environmental impacts, monitoring and modeling methodologies I. In *AGU Fall Meeting 2019.* AGU.

Cesar, J., Nightingale, M., Becker, V., & Mayer, B. (2019, September). Organic and isotope geochemistry of a hybrid petroleum system. In *29th International Meeting on Organic Geochemistry (Vol. 2019, No. 1, pp. 1-2).* European Association of Geoscientists & Engineers.

Cesar, J., Nightingale, M., Becker, V., & Mayer, B. (2019, May) Organic and isotope geochemistry of hybrid hydrocarbon accumulations. In *GeoConvention 2019.*

Cesar, J., Nightingale, M., Becker, V., & Mayer, B. (2019, August). The isotope fingerprint of hydrocarbons from hybrid accumulations. In *Goldschmidt 2019 Abstracts (509).* The European Association of Geochemistry.

Chen, H., & Innanen, K. A. (2018). Seismic amplitude difference inversion for fracture weaknesses and attenuation factors. In *SEG Technical Program Expanded Abstracts 2018 (pp. 291-295).* Society of Exploration Geophysicists.

Cova, R., Innanen, K., & Rauch-Davies, M. (2019, June). Pre-processing a land walkaway VSP dataset for elastic FWI: Effects of deconvolution operations. In *81st EAGE Conference and Exhibition 2019 (Vol. 2019, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Eaton, D., Mahani, A., salvage, R., Kao, H., & van der Baan, M. (2019, October) A tale of three earthquakes: New insights into fault activation in light of recent occurrences in Western Canada. In *2019 William C. Gussow Geoscience Conference.* Canadian Society of Petroleum Geologists.

Esmaeili, S., Sarma, H., Harding, T., & Maini, B. (2019, September). The effect of temperature on two-phase oil/water relative permeability in different rock/fluid systems. In *SPE Annual Technical Conference and Exhibition.* Society of Petroleum Engineers.

Eyre, T. S., Eaton, D. W., & Tyrrell, T. (2018). Persistent post-injection induced seismicity near Fox Creek, Alberta. In *SEG Technical Program Expanded Abstracts 2018 (pp. 4982-4986).* Society of Exploration Geophysicists.

Eyre, T., Eaton, D. W., Garagash, D., Zecevic, M., Venieri, M., Weir, R., & Lawton, D. C. (2019). Hydraulic-fracturing induced seismicity driven by aseismic creep. In *AGU Fall Meeting 2019 (T33A-03).*

Eyre, T. (2019, May). Advanced simulation environment for induced seismicity mitigation and integrated control (ASEISMIC). In *GeoConvention 2019.*

Eyre, T. (2019, May). Implications of long-lived post-injection induced seismicity near Fox Creek, Alberta. In *GeoConvention 2019.*

Fleming, N., Morais, T., Kennedy, C., & Ryan, C. (2019, May). Evaluation of SCVF and GM measurement approaches to detect fugitive gas migration around energy wells. In *GeoConvention 2019.*

Forde, O. N., Mayer, U. K., Cahill, A. G., Beckie, R. D., & Mayer, B. (2019). Fugitive gas migration and effluxes at oil and gas sites. In *2019 AGU Fall Meeting, H54B-04.* American Geophysical Union.

Gilbert, H. J., Savard, G., Macquet, M., Lawton, D. C., & Gu, Y. J. (2019, December). Passive seismic monitoring at the CaMI Field Research Station, Alberta, Canada. In *AGU Fall Meeting 2019.* American Geophysical Union.

Goodarzi, S., Lawton, D., & Osadetz, K. (2019, April). Coupled fluid flow modeling in the wellbore and reservoir for CO_2 injection at the CaMI Field Research Station. In *Proceedings of the 4th World Congress on Momentum, Heat and Mass Transfer* (MHMT'19) (ENFHT 141).

Harazim, D., Pedersen, P., Zappi, A., Guevara, O., Figueroa, E. V., Rivera, I. D. J. H., Morales, S. C., & Vargas, R. T. (2019, May) Predicting reservoir connectivity within ancient coastal plain systems during exploration, appraisal and development — Pitfalls and best practices. In *2019 AAPG Annual Convention and Exhibition.*

Hui, G., Chen, S., Chen, Z., & Eaton, D. (2019, August). An integrated approach to characterize the induced seismicity triggered by hydraulic fracturing in Duvernay reservoir. In *53rd US Rock Mechanics/ Geomechanics Symposium.* American Rock Mechanics Association.

Karamad, M., Siahrostami, S., & Gates, I. D. (2019, October). Doped transition metal nitrides as efficient electrocatalysts for electrochemical reduction of CO_2. In *236th ECS Meeting (1088).* ECS.

Kazemi, N., Trad, D., Innanen, K., & Shor, R. (2019, June). Joint least-squares RTM of surface seismic and seismic-while-drilling datasets. In *81st EAGE Conference and Exhibition 2019 (Vol. 2019, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Keating, S., & Innanen, K. A. (2018). Strategies for reducing cross-talk in visco-acoustic full-waveform inversion. In *SEG Technical Program Expanded Abstracts 2018 (pp. 1218-1222).* Society of Exploration Geophysicists.

Kelly, S., Siahrostami, S., & Nørskov, J. K. (2019, June). Successes and outlooks for modeling 2-electron water oxidation to H_2O_2. In *2019 North American Catalysis Society Meeting.* NAM.

Kloppmann, W., Mayer, B., Humez, P., Osselin, F., Eric, G., Blessing, M., Gal, F., Desaulty, A-M., Guerrot, C., Lerouge, C., Innocent, C., & Millot, R. (2019, November). Comment évaluer l'impact de l'exploration et l'exploitation de gaz non conventionnels: Traçage multi-isotopique des fluides salins et des gaz. In *SFIS2019–7ème congrès de la Société Française des Isotopes.*

Larter, S., Radovic, J. R., Silva, R. C., & De La Fuente, J. (2019, August) Geoengineering the carbon cycles in the ocean. In *Goldschmidt 2019 Abstracts (1829).* The European Association of Geochemistry.

Li, Q., Aguilera, R., & Cinco-Ley, H. (2019). A correlation for estimating the Biot coefficient. *SPE Drilling & Completion.*

Macquet, M., & Lawton, D. (2018, November). Reservoir simulation and feasibility study for seismic monitoring at CaMI. FRS, Newell County, Alberta. In *Fifth CO2 Geological Storage Workshop (Vol. 2018, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Macquet, M., Lawton, D., Savard, G., & Gilbert, H. J. (2019). Exploring ambient noise correlation technique for monitoring CO_2 injection at the CaMI Field Research Station. In *AGU Fall Meeting 2019* (S34B-03).

Manasrah, A. D, N. N. Nassar Conversion of petroleum coke into value-added products using oxy-cracking technology, AEAB2019 — *Applied Energy Symposium: MIT A+B*, Boston, USA, May 22-24, 2019.

Mayer, B., Humez, P., Osselin, F., Nightingale, M., Becker, V., Saad, S., MacDonald, M., Cesar, J. & Kloppmann, W. (2019). A toolbox for the accurate detection of the sources of fugitive methane associated with development of unconventional hydrocarbon resources. *AGU Fall Meeting 2019* (H51J-1609).

Marei, N. N., Kibria, M. G., & Shimizu, G. K. (2019, November). An integrated CO_2 capture and conversion device based on metal-organic framework-and Cu nanostructured electrocatalyst. In *2019 AIChE Annual Meeting.* AIChE.

Nejadi, S., Curkan, J. A., Durkin, P. R., Hubbard, S. M., & Gates, I. D. (2019, September). Integrated reservoir characterization and multiscale heterogeneity modeling of stacked Meander-belt deposits, Lower Cretaceous McMurray Formation, Alberta. In *Petroleum Geostatistics 2019* (Vol. 2019, No. 1, pp. 1-5). European Association of Geoscientists & Engineers.

Nejadi, S., Kazemi, N., Hubbard, S. M., & Gates, I. D. (2019, March). A Bayesian sampling framework with seismic priors for data assimilation and uncertainty quantification. In *SPE Reservoir Simulation Conference.* Society of Petroleum Engineers.

Olusola, B., Aguilera, R., and Cinco-Ley H. (2020). Incorporating Biot Poroelastic Coefficient on Pickett Plots. Paper SPE -198959 — MS presented at the *Virtual SPE Latin American and Caribbean Petroleum Engineering Conference* (LACPEC) held on 27-31 July 2020.

Pang, Y., Fan, D., & Chen, S. (2020, July). A novel approach to determine gas velocity profile in entire Knudsen number regime for nanoporous shale with various pore geometries. In *SPE/AAPG/SEG Unconventional Resources Technology Conference.* Unconventional Resources Technology Conference.

Radovic, J. R., Novotnik, B., Venkatesan, S., Thangadurai, V., Strous, M., & Larter, S. (2019, August) The future of petroleum resources: From fuels to electricity? In *Goldschmidt 2019 Abstracts (2749).* The European Association of Geochemistry.

Savard, G., Bostock, M. G., Hutchinson, J. A., Kao, H., Christensen, N. I., & Peacock, S. M. (2019). Plate deformation at Cascadia's Northern Terminus. In *AGU Fall Meeting 2019* (T14B-03).

Siahrostami, S. (2019, March). Electrochemical synthesis of hydrogen peroxide via different routes. In *Abstracts of Papers of the American Chemical Society (Vol. 257).* American Chemical Society.

Siahrostami, S. (2019, May). Oxygen reduction reaction, catalyst development. In *235th ECS Meeting (May 26-30, 2019).* ECS.

Sibaweihi, N., Patel, R. G., Guevara, J. L., Gates, I. D., & Trivedi, J. J. (2019, April). Real-time steam allocation workflow using machine learning for digital heavy oil reservoirs. In *SPE Western Regional Meeting.* Society of Petroleum Engineers.

Soares, J. V., Chopra, C., Mayer, K. U., Cahill, A., Beckie, R. D., Black, A., Mayer, B., Chao, J., Manning, C., & Cary, T. (2019, September). Transport of fugitive gas to the vadose zone and atmosphere during a controlled release of natural gas into an aquifer in northeastern British Columbia, Canada. In *GSA Annual Meeting in Phoenix, Arizona, USA-2019.* Geological Society of America.

Thangadurai, V., & Mulmi, S. (2019, May). Solid state electrochemical gas sensors: Fundamentals, materials and applications. In *235th ECS Meeting (May 26-30, 2019).* ECS.

Venkatesan, S. V., Abubaker, O. A., Singh, K., & Thangadurai, V. (2019, October). Cobalt-free perovskite-type oxygen reduction reaction catalysts for energy conversion. In *236th ECS Meeting (October 13-17, 2019).* ECS.

Wei, W., Wang, J., & Gates, I. (2019, June). New insights into Kerrobert Toe-to-Heel Air Injection (THAI) production analysis. In *81st EAGE Conference and Exhibition 2019 (Vol. 2019, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Wu, C., & Gates, I. (2019, August). Methane activation by an iron atom supported on graphene. In *Abstracts of Papers of The American Chemical Society (Vol. 258).* American Chemical Society.

Wu, C., Liu, D., Chen, Q., & Gates, I. (2019, August). Activity-tunable biocatalyst for algal cell wall degradation and lipids extraction. In *Abstracts of Papers of The American Chemical Society (Vol. 258).* American Chemical Society.

Zargartalebi, M., & Benneker, A. (2019). Optimization of porous medium structure to enhance heat transfer in microchannel. *APS,* G38-004.

Zhang, Z., Singh, K., & Thangadurai, V. (2019, October). Investigating phase and electrical properties of calcium-doped yttrium iron garnet. In *236th ECS Meeting (October 13-17, 2019).* ECS.

Abboud, J. M., & Ryan, M. C. (2018, May) Is the rate of fugitive methane gas migration around Alberta's energy wells adequately estimated? In *GeoConvention 2018.*

Abboud, J. M., & Ryan, M. C. (2018, September) Is the rate of fugitive methane gas migration around Alberta's energy wells adequately constrained? In *GeoEdmonton 2018.*

Abboud, J. M., Ryan, M. C., Hayley, J. L. & Lauer, R. M. (2018, September) Pressure redistribution and free phase gas formation during and after undrained unloading of dissolved gas-charged sediment. In *GeoEdmonton 2018.*

Cahill, A. G., Sandl, E., Chao, J., Goetz, M., Soares, J., Cary, T.,Hawthorne, I., Finke, N., Manning, C., Ladd, B., Welch, L. A., Black, T. A., Lauer, R. M., Mayer, U. K., Crowe, S., Mayer, B., Kirste, D. M. & Beckie, R. D. (2018, December). Investigating gas leakage from oil and gas wells in NE BC, Canada through statistical analysis of occurrence, regional hydrogeological field investigations and controlled subsurface natural gas release experiments. In *AGU Fall Meeting 2018,* H14B-07.

Cova, R., Henley, D., & Innanen, K. A. (2018). Computing near-surface velocity models for S-wave static corrections in the τ-p domain. In SEG Technical *Program Expanded Abstracts 2018 (pp. 2402-2406).* Society of Exploration Geophysicists.

Eaid, M., Li, J., & Innanen, K. A. (2018). Modeling the response of shaped-DAS fibres to microseismic moment tensor sources. In *SEG Technical Program Expanded Abstracts 2018 (pp. 4698-4702).* Society of Exploration Geophysicists.

Gal, F., Proust, E., Humez, P., Mayer, B., Gaucher, E., & Kloppmann, W. (2018, April). Soil gas flux measurements as part of environmental baseline assessment. In *EGU General Assembly Conference Abstracts* (Vol. 20, p. 8599).

Goodarzi, S., Vishkai, M., Soroush, M., & Gates, I. D. (2018, August). Geostatistical modeling accounting for variation of reservoir and geomechanical properties in Montney Formation, Alberta. In *52nd US Rock Mechanics/Geomechanics Symposium.* American Rock Mechanics Association.

Gordon, A., & Lawton, D. C. (2018, May). VSP processing of Distributed Acoustic Sensing and geophone data at CaMI Field Research Station, Newell County, Alberta. In *GeoConvention 2018.*

Gordon, A., Lawton, D., Hall, K., Freifeld, B., Daley, T., & Cook, P. (2018). Depth registration of VSP DAS fiber. In *SEG Technical Program Expanded Abstracts 2018 (pp. 5427-5431).* Society of Exploration Geophysicists.

Hall, K. W., Lawton, D. C., Daley, T. M., Freifeld, B. M., & Cook, P. (2018, May). Effect of source effort and source distance on DAS data at CaMI. FRS, Newell County, Alberta. In *GeoConvention 2018.*

Hall, K.W., Lawton, D.C., Daley, T.M., Freifeld, B.M., Marchesini, P., Cook, P. (2018) Effect of source effort and source distance on optical fibre data at CaMI.FRS, Newell County, Alberta. In *2018 SEG International Exposition and Annual Meeting (pp. 206-210).* Society of Exploration Geologists.

Hosseinabad, F. S., Yasri, N., Roesler, R., Maslovara, S., Roberts, E. (2018, July). An iodide-based complexing agent for the zinc-iodide flow battery. In *AiMES 2018 Meeting Abstracts (No. 1, pp. 33-33).* The Electrochemical Society.

Hwang, D. H., Do, H., Jun, S. C., Lee, K. K., Shevallier, M., Mayer, B., & Yun, S. T. (2018). Geochemical change of groundwater by artificial CO_2 leakage through shallow silicate aquifer: emphasis on pH buffering. In *AGU Fall Meeting 2018* (MR53A-0097).

Innanen, K. A. (2018). Potential monitoring applications of seismic reflections from time and mixed space/time boundaries. In *SEG Technical Program Expanded Abstracts 2018 (pp. 3868-3872).* Society of Exploration Geophysicists.

Innanen, K., & Eaid, M. (2018, June). Towards discrimination of elastic wave modes with shaped DAS fibre-optic cables. In *80th EAGE Conference and Exhibition 2018 (Vol. 2018, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Iverson, A., Innanen, K. A., & Trad, D. (2018). Internal multiple prediction in the offset-time domain: Response to irregular spatial sampling. In *SEG Technical Program Expanded Abstracts 2018 (pp. 4538-4542).* Society of Exploration Geophysicists.

Kazemi, N., Shor, R., & Innanen, K. (2018). Imaging with a seismic-while-drilling dataset. In *Proc. CSPG CSEG CWLS Conv.* (pp. 1-4).

Kazemi, N., Shor, R., & Innanen, K. (2018, June). Illumination compensation with seismic-while-drilling plus surface seismic imaging. In *80th EAGE Conference and Exhibition 2018 (Vol. 2018, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Kazemi, N., Shor, R., & Innanen, K. (2018, June). Imaging with a seismic-while-drilling dataset. In *80th EAGE Conference and Exhibition 2018 (p. 1-5).* European Association of Geoscientists & Engineers.

Laventure, A., Harding, C. R., Cieplechowicz, E., & Welch, G. C. (2018, September). Towards upscaling of organic photovoltaics using non-fullerene acceptors. In *Organic, Hybrid, and Perovskite Photovoltaics XIX (Vol. 10737, p. 107370H).* International Society for Optics and Photonics.

Lawton, D., Hall, K., & Gordon, A. (2018). Advances in DAS seismic monitoring for CO_2 storage. In *SEG Technical Program Expanded Abstracts 2018 (pp. 5500-5500).* Society of Exploration Geophysicists.

Li, J., Fofana, D., Li, X., El-Sawy, E., Birss, V., Hosseinabad, F. S., Maslovara, S., Roberts, E. P. (2018). A nano-carbon scaffold (NCS) electrode for the vanadium redox flow battery. In *233rd Electrochemical Society Meeting Abstracts (No. 41, pp. 2386-2386).* ECS.

Li, J., Innanen, K. A., Pan, W., & Yu, G. (2018). Frequency domain elastic FWI for VTI media. In *SEG Technical Program Expanded Abstracts 2018 (pp. 1223-1227).* Society of Exploration Geophysicists.

Li, J., Innanen, K. A., & Tao, G. (2018). A 3D pseudo-spectral method for SH wave simulation in heterogeneous media. In *SEG Technical Program Expanded Abstracts 2018 (pp. 4005-4009).* Society of Exploration Geophysicists.

Li, S. and Du, K. (2018). Quantification of fugitive area methane emission using multi-path optical remote sensing and dispersion modeling method. In *Proceedings of the Air and Waste Management Association's 111th Annual Conference and Exhibition.* AWMA.

Macquet, M., & Lawton, D. (2018). CaMI Field Research Station, Alberta, Canada: Feasibility study for time lapse seismic monitoring and ambient noise correlation. In *AGU Fall Meeting 2018* (S54A-06).

Macquet, M., & Lawton, D. (2018, November). Reservoir simulation and feasibility study for seismic monitoring at CaMI. FRS, Newell County, Alberta. In *Fifth CO_2 Geological Storage Workshop (Vol. 2018, No. 1, pp. 1-5).* European Association of Geoscientists & Engineers.

Macquet, M., & Lawton, D. (2018, May) Reservoir simulations and feasibility study for seismic monitoring at CaMI.FRS, Newell County, Alberta. In *Geoconvention 2018.*

Mayer, B., Humez, P., Osselin, F., Cheung, T., Becker, V., Parker, B., Cherry, J., Nightingale, M., Clarkson, C., Wolfram, K., Gaucher, E., Osadetz, K. & Lawton, D. (2018, April). A comprehensive approach for assessing potential fugitive gas migration associated with petroleum development from low permeability reservoirs: case studies from Western Canada. In *EGU General Assembly Conference Abstracts* (Vol. 20, p. 5634).

McKean, S. H., Priest, J. A., Eaton, D. W. (2018). A geomechanical comparison of the Duvernay and the Montney. In *GeoConvention 2018.*

McKean, S. H., Priest, J. A., Eaton, D. W., Philips, J., van der Baan, M. (2018). An industry perspective on induced seismicity. In *Geoconvention 2018.*

McKean, S. H., Priest, J. Dettmer. J. A., Eaton D. W. (2018). Identifying discrete fracture networks from microseismic data using clustering. In *GeoEdmonton 2018.*

Mohammadmoradi, P., & Kantzas, A. (2018, March). Longitudinal dispersion coefficient in consolidated porous media; a pore-level study. In *SPE Canada Heavy Oil Technical Conference.* Society of Petroleum Engineers.

Mohammadmoradi, P., & Kantzas, A. (2018, March). Wettability and capillary imbibition in shales; analytical and data-driven analysis. In *SPE Canada Unconventional Resources Conference.* Society of Petroleum Engineers.

Mohammadmoradi, P., Moradi, H. M., & Kantzas, A. (2018, April). Data-driven production forecasting of unconventional wells with apache spark. In *SPE Western Regional Meeting.* Society of Petroleum Engineers.

Moradi, S., Trad, D., & Innanen, K. A. (2018). Quantum computing in geophysics: Algorithms, computational costs, and future applications. In *SEG Technical Program Expanded Abstracts 2018 (pp. 4649-4653).* Society of Exploration Geophysicists.

Nejadi, S., Hubbard, S. M., Shor, R. J., Gates, I. D., & Wang, J. (2018, November). Optimization of placement of flow control devices under geological uncertainty in steam assisted gravity drainage. In *SPE Thermal Well Integrity and Design Symposium.* Society of Petroleum Engineers.

Osadetz, K.G., Mort, A., Snowdon, L.R., Lawton, D.C, Chen, Z., and Saeedfar, A., (2018, May). Western Canada Sedimentary Basin petroleum systems: Where is the secondary biogenic gas? In *Geoconvention 2018.*

Riley, D. J. T., Mayer, B., Nightingale, M., Shevalier, M., Lawton, D. C., & Osadetz, K. (2018). Characterizing baseline soil gas conditions at the Containment and Monitoring Institute (CaMI) CO_2 Injection Site in Alberta, Canada. In *AGU Fall Meeting, 2018,* H23P-2186.

Rippe, D., Jordan, M., Romdhane, A., Schmidt-Hattenberger, C., Macquet, M., & Lawton, D. (2018). Accurate CO_2 monitoring using quantitative joint inversion at the CaMI Field Research Station (FRS), Canada. In *14th International Conference on Greenhouse Gas Control Technologies-GHGT-14.*

Silva, R., Pedersen, J. H., di Primio, R., Snowdon, L., Huang, H., Larter, S., & Norway-Norway, L. (2018, May). Routes and progress in age dating fluid residence time in subsurface reservoirs: Issues and E&P Applications. In *GeoConvention 2018.*

Spackman, T. W., & Lawton, D. C. (2018, May) Seismic monitoring with continuous seismic sources. In *GeoConvention 2018.*

Spackman, T. W., & Lawton, D. C. (2018). Analysis of distributed acoustic sensing and geophone VSP data for continuous seismic source studies. In *SEG Technical Program Expanded Abstracts 2018 (pp. 4943-4947).* Society of Exploration Geophysicists.

Tawiah, P., Duer, J., Bryant, S., Larter, S., OBrien, S., & Dong, M. (2018, October). CO_2 injectivity behaviour-field observations from the quest CCS operations. In *14th Greenhouse Gas Control Technologies Conference Melbourne* (pp. 21-26).

Vishkai, M., & Gates, I. D. (2018, August). Geomechanical characterization of naturally fractured formation, Montney, Alberta. In *52nd US Rock Mechanics/Geomechanics Symposium.* American Rock Mechanics Association.

Weir, R., Lines, L., Lawton, D., & Eyre, T. (2018). The Duvernay Formation: the application of structure and simultaneous inversion for reservoir characterization and induced seismicity. In *SEG Technical Program Expanded Abstracts 2018 (pp. 2372-2376).* Society of Exploration Geophysicists.

Eaton, D. (2017, June). Dynamics of fault activation by hydraulic fracturing in overpressured shales. In *79th EAGE Conference and Exhibition 2017-Workshops (pp. cp-519).* European Association of Geoscientists & Engineers.

Eyre, T., & Eaton, D. W. (2017). Microseismic data records fault activation before and after a M w 4.1 induced earthquake. In *AGU Fall Meeting 2017 (S23C-0847).*

Larter, S., Silva, R. C., Snowdon, L., Marcano, N., Huang, H., Villareal, E., Zhao, J., Sonei, R., Gutierrez, L. P., Pedersen, J. H., di Primio, R. (2017) The dating of fluid residence time in subsurface reservoirs. Challenges, strategies and a design schematic for a practical geochemical toolbox. In *CSPG Gussow Conference.*

Osselin, F., Nightingale, M., Kloppmann, W., Gaucher, E., Clarkson, C., & Mayer, B. (2017). Quantifying water-rock interactions during hydraulic fracturing from the analysis of flowback water. In *AGU Fall Meeting 2017 (B11B-1666).*

Zhan, J., Han, Y., Fogwill, A., Wang, K., Hejazi, H., He, R., & Chen, Z. (2017, November). A novel integrated numerical simulation scheme for transient gas flow in shale matrix. In *SPE Symposium: Production Enhancement and Cost Optimisation.* Society of Petroleum Engineers.

Zhan, J., Yuan, Q., Fogwill, A., Cai, H., Hejazi, H., Chen, Z., & Cheng, S. (2017, August). A systematic reservoir simulation study on assessing the feasibility of CO_2 sequestration in shale gas reservoir with potential enhanced gas recovery. In *Carbon Management Technology Conference*. Carbon Management Technology Conference.

Book chapters

Lawton, D., Dongas, J., Osadetz, K., Saeedfar, A., & Macquet, M. (2019). Development and analysis of a geostatic model for shallow CO_2 injection at the Field Research Station, Southern Alberta, Canada. In *T. Davis, M. Landrø, & M. Wilson (Eds.), Geophysics and Geosequestration (pp. 280-296).* Cambridge: Cambridge University Press.

Mulmi, S., & Thangadurai, V. (2019). Solid-state electrolytes: Structural approach. In *R. Murugan, & W. Weppner (Eds.), Solid Electrolytes for Advanced Applications (pp. 3-24).* Springer, Cham.

Huang H., Silva R. C., Radović J. R., and Larter S. R. (2018). Environmental and economic implications of the biogeochemistry of oil sands bitumens. In *Wilkes H. (Ed.), Hydrocarbons, Oils and Lipids: Diversity, Origin, Chemistry and Fate.* Handbook of Hydrocarbon and Lipid Microbiology. Springer International Publishing AG, part of Springer Nature 2018.

Radović, J. R., Oldenburg, T. B., & Larter, S. R. (2018). Environmental assessment of spills related to oil exploitation in Canada's oil sands region. In *S. A. Stout, & Z. Wang (Eds.) Oil Spill Environmental Forensics Case Studies (pp. 401-417).* Butterworth-Heinemann.

Conference presentations

Ai, C., Li, X., Mayall, R., & Birss, V. (2020, January 26-31). Scalable *nanoporous carbon scaffolds for ultrafiltration applications. 2020 Chemical Separations,* Gordon Research Conference, Galveston, TX, United States.

Paterson, A., Goetzee-Barral, A., Johnson, A. N., Bell, A. J., & Dolgos, M. (2020, January 22-24). *Length scale dependence of the structure of (1-x) Na Bi TiO -xPbTiO via pair distribution functions*. Electronic Materials and Applications 2020, Orlando, FL, United States.

Rana, M., Xu, J. & De la Hoz Siegler, H. (2020, January 17-20) *Synthesis-solvent effects on the properties of smart hydrogels*. 8th International Conference on Nano and Materials Science ICNMS 2020, Seattle, WA, United States.

Bhoria, N. (2019, June 11-13) *Carbon-dioxide conversion into high-value fuels and feedstocks using metal-organic frameworks based electrocatalyst*. Global Petroleum Show 2019, Calgary, AB, Canada.

Bhoria, N., & Kibria, M. G. (2019, October 20-23). *Selective carbon-dioxide electro-reduction to C2+ products using multi-metallic MOFs*. 69th Canadian Chemical Engineering Conference, Halifax, NS, Canada.

Bhoria, N., & Kibria, M. G. (2019, May 02-03). *Nanostructured MOF catalysts for electrochemical reduction of carbon dioxide*. 6th Alberta Nano Research Symposium, Edmonton, AB, Canada.

Bryant, S. (2019, December 05). *Negative emissions technologies with energy production: can Canada's oil & gas industry help reverse climate change?* CSPG Technical Luncheon & geoLOGIC Holiday Social, Calgary, AB, Canada.

Calderon, O., Birss, V., & Trudel, S. (2019, June 3-7) *Towards in operando XAS investigation of CO_2 electrolysis in Solid Oxide Cells: Effect of Sr and Ca doping in $LaCrFeO_{3-\delta}$ perovskites*. 102nd Canadian Chemistry Conference and Exhibition, Québec City, QC, Canada.

Cavanzo Balcazar, E. A., Schoeggl, F. F., Yarranton, H. W., & Kantzas, A. (2019, October 20-23) *Solvent diffusion in a solvent/water/bitumen system*. 69th Canadian Chemical Engineering Conference, Halifax, NS, Canada.

Cieplechowicz, E., & Welch, G. (2019, June 1-7) *Structure modification of perylenediimides (pdi) for application in indoor photovoltaics*. 14th International Symposium on Functional ϖ-Electron Systems, Berlin, Germany.

Demirkaya, C., Tervahauta, T., Vadlamani, A., Strous, M., & De la Hoz Siegler, H. (2019, June 17-19) *Enhancing biogas production from algae by integration of autofermentation and anaerobic digestion*. 9th International Conference on Algal Biomass, Biofuels, and Bioproducts, Boulder, CO, United States.

Dolgos, M. (2019, January 23) *Accidental discoveries of relaxor ferroelectrics*. Electronic Materials and Applications 2019, The American Ceramic Society, Orlando, FL, United States. [Invited talk]

Dolgos, M. (2019, July 14-19). *Using simple aqueous precursors to synthesize potassium sodium Niobate thin films*. 2019 IEEE International Symposium on Applications of Ferroelectrics (ISAF), Lausanne, Switzerland.

Eaton, D. (2019, October 17) *The role of aseismic slip in hydraulic fracturing–induced seismicity*. Canadian Society for Unconventional Resources (CSUR) Induced Seismicity Workshop V, Calgary, AB, Canada.

Eyre, T., & Eaton, D. (2019, November 12-14). *The role of aseismic slip in hydraulic fracturing–induced seismicity.* SPE/SEG Workshop: Injection Induced Seismicity — The Next Chapter, Dallas, TX, United States.

Eyre, T. (2019, June 26). *Implications of persistent post-injection induced seismicity in the Duvernay.* CSEG Lunchbox Geophysics, Calgary, AB, Canada.

Eyre, T. (2019, May 13-17). *Advanced simulation environment for induced seismicity mitigation and integrated control (ASEISMIC).* GeoConvention 2019, Calgary, AB, Canada.

Eyre, T. (2019, May 13-17). *Implications of long-lived post-injection induced seismicity near Fox Creek, Alberta*. Geoconvention 2019, Calgary, AB, Canada.

Eyre, T. (2019, April 24-26). *Advances, developments and future research into seismicity in natural and anthropogenic fluid-driven environments*. Seismological Society of America Annual Meeting, Seattle, WA, United States.

Fleming, N., Morais, T., Kennedy, C., & Ryan, C. (2019, May 13-17). *Evaluation of SCVF and GM measurement approaches to detect fugitive gas migration around energy wells*. Geoconvention 2019, Calgary, AB, Canada.

Gao, M., Fox, T. A., Barchyn, T. E., & Hugenholtz, C. H. (2019, November 26-27). *Drone-based methane sensing — operational reliability moderated by weather.* 2019 Methane Emissions Reduction Forum, Banff, AB, Canada.

Goodarzi, S., Osadetz, K., & Lawton, D. (2019, June 11-13). *Coupled fluid flow modeling in the wellbore and reservoir for CO_2 injection at the CaMI (Containment and Monitoring Institute) Field Research Station.* Global Petroleum Show 2019, Calgary, AB, Canada.

Hannouf, M., Assefa, G., & Gates, I. (2019, September 24-26). *Social life cycle assessment for technologies in early stage of development: The case of oil and technologies*. American Centre of Life Cycle Assessment, LCA XIX, Tucson, AZ, United States.

Hugenholtz, C., & Fox, T. (2019, November 26-27). *Intelligent methane monitoring & management system (IM3S): Reducing methane emissions with advanced analytics*. Petroleum Technology Alliance of Canada: Methane Emissions Reduction Forum, Banff, AB, Canada.

Karimi, F., Alihosseinzadeh, A., Ponnurangam, S., & Karan, K. (2019, July 02-05). *Performance characteristics of gas-fed CO_2 electrolysis on silver nanoparticles in alkaline exchange membrane electrode assembly.* European Fuel Cell Forum Conference, Lucerne, Switzerland.

Kibria, M. G. (2019, October 20-23) *Artificial photosynthesis for sustainable energy and environment: lessons learned and the paths forward*. 69th Canadian Chemical Engineering Conference, Halifax, NS, Canada.

Martinez, F., Ponnurangam, S., & Birss, V. I. (2019, June 03-07). *Computational study of the structure and properties of perovskites-based solid oxides for CO_2 conversion at high temperature*. 102nd Canadian Chemistry Conference and Exhibition, Québec City, QC, Canada.

McQuade, R., Manjon-Sanz, A., Rowe, T., de la Puente, L., Smith, S., & Dolgos, M. (2019, July 31-August 02). *Structure-property relationships in modified $Na_{0.5}Bi_{0.5}TiO_3$-$BaTiO_3$ piezoelectrics*. 2019 North American Solid State Chemistry Conference, Golden, CO, United States.

Mendiratta, S., Hejazi, H., De la Hoz Siegler, H., Natale, G., Lu, Q., & Gates, I.D. (2019, January 27-29) *Synthesis, characterization, and functionalization of hydroxyapatite nanoparticles*. International Conference on Advances in Nanomaterials and Devices for Energy and Environment (ICAN-2019), Gwalior, India.

Mohsin, I., Sumon, K. Z., McCoy, S. T., & Kibria, M. G. (2019, October 20-23). *Techno-economic and life-cycle assessment of an integrated carbon capture and conversion process for sustainable production of high-value fuels and feedstocks*. 69th Canadian Chemical Engineering Conference, Halifax, NS, Canada.

Mohsin, I., & Kibria, M. G. (2019, June 11-13). *An integrated carbon capture & conversion plant*. Global Petroleum Show 2019, Calgary, AB, Canada.

Nandy, A., Novotnik, B., Radovic, J. R., Venkatesan, S. V., & Thangadurai, V., Larter, S. R., & Strous, M. (2019, October 07-14). *Microbial Fuel Cells: A climate neutral technology for direct electricity production from crude oil*. 7th International Society for Microbial Electrochemistry and Technology Conference, Okinawa, Japan.

Novotnik, B., Radovic, J., Nandy, A., Larter, S., & Strous, M. (2019, June 18-21). *Microbial metal dependent conversions of hydrocarbons for zero CO2 emission energy extraction*. 7th International Symposium on Applied Microbiology and Molecular Biology in Oil System, Halifax, NS, Canada.

Paquette, A., Vadlamani, A., Strous, M., De la Hoz Siegler, H. (2019, October 20-23) *The new tradition is good nutrition: comprehensive analysis of nutrient assimilation in alkaliphilic cyanobacteria*. 69th Canadian Chemical Engineering Conference, Halifax, NS, Canada.

Rana, M., & De la Hoz Siegler, H. (2019, October 20-23) *Development of smart hydrogels with tunable properties for biomedical and environmental applications.* 69th Canadian Chemical Engineering Conference, Halifax, NS, Canada.

Rowe, T., Topham, D., & Dolgos, M. (2019, January 23-25). *(1-x)NaNbO3-(x)BaZrO3 perovskites to discover a novel relaxor ferroelectric material.* Electronic Materials and Applications 2019, The American Ceramic Society, Orlando, FL, United States.

Siahrostami, S. (2019, August 25-29). *Electrochemical synthesis of hydrogen peroxide for water treatment.* American Chemical Society Fall 2019 National Meeting & Expo, San Diego, CA, United States.

Siahrostami, S. (2019, June 03-06). *Electrochemical synthesis of hydrogen peroxide for onsite water treatment.* 102nd Canadian Chemistry Conference and Exhibition, Québec City, QC, Canada.

Singh, K., Abubaker, O. A., Baral, A. K., Weinfeld, K., Tsur, Y., & Thangadurai, V. (2019, June 03-07). *Origin and effect of chemical capacitance on oxygen reduction reaction in Cu-doped $Ba_{0.5}Sr_{0.5}Fe_{1-x}Cu_{x}O_{3-\delta}$, studied by impedance spectroscopy genetic programming.* 102nd Canadian Chemistry Conference and Exhibition, Québec City, QC, Canada.

Song P., & Lu Q. (2019, July 28-August 01). *Buckling effect of sole ZIF-8 nanoparticles adsorbed at the water/oil interface.* The 17th National Symposium of Colloids and Interfaces, Wuxi, China.

Suri, N., Gieg, L., & Ryan, C. (2019, June 18-21). *In situ microbial gas production: geomechanical implications and oil displacement.* 7th International Symposium on Applied Microbiology and Molecular Biology in Oil System, Halifax, NS, Canada.

Vadlamani, A., Demirkaya, C., Zorz, J., Paquette, A., Ataeian, M., De la Hoz Siegler, H., & Strous, M. (2019, October 20-23) *Cyanobacterial consortium cultivation using atmospheric CO_2 and phycocyanin production.* 69th Canadian Chemical Engineering Conference, Halifax, NS, Canada.

Wang, M., & Kibria, M. G. (2019, October 20-23). *Techno-economic analysis of electrochemical ammonia synthesis.* 69th Canadian Chemical Engineering Conference, Halifax, NS, Canada.

Willkomm, J., Bertin, E., Atwa, M., Lin, J., Birss, V., & Piers, W. E. (2019, June 03-07). *Grafting of a molecular rhenium CO_2 reduction catalyst onto colloid-imprinted carbon.* 102nd Canadian Chemistry Conference and Exhibition, Québec City, QC, Canada.

Zanca, B., & Dolgos, M. (2019, January 23-25) *Structure-property relationships of alkali and alkaline earth substituted bismuth pyrostannate (Bi2-xMxSn2O7).* Electronic Materials and Applications 2019, The American Ceramic Society, Orlando, FL, United States.

Abubaker, O., Singh, K., Thangadurai V. (2018, May 27-31). *Effect of Cu doping on the oxygen reduction reaction properties of $Ba_{0.5}Sr_{0.5}Fe_{1-x}Cu_{x}O_{3-\delta}$ cathodes.* Canadian Society for Chemistry 101st Canadian Chemistry Conference and Exhibition, Edmonton, AB, Canada.

Caceres-Falla, M., & De la Hoz Siegler, H. (2018, October 28-31). *Atmospheric CO_2 capture in carbonate/bicarbonate solution for autotrophic microalgae.* 68th Canadian Chemical Engineering Conference, Toronto, ON, Canada.

Chernyshova, I.V., Somasundaran, P., & Ponnurangam, S. (2018, August 19-23). *The origin of the elusive first intermediate of CO_2 electroreduction.* 256th American Chemical Society National Meeting, Boston, MA, United States.

Eaton, D. W., Eyre, T.S., McKean, S., Gang, H., Chen, N., & Priest, J. (2018, June 12-14). *Mitigating and managing risks of induced seismicity caused by hydraulic fracturing.* Global Petroleum Show, Calgary, AB, Canada.

Goodarzi, S., Saeedfar, S., Osadetz, K., & Lawton, D. (2018, May 25). *Overview of the injection and monitoring activities in the Field Research Station (FRS), Newell County, Alberta, Canada.* The 2018 Research Experience in Carbon Sequestration Program, Birmangham, AL, United States.

Hugenholtz, C. (2018, November 27-28). *Equivalent emissions reduction: What does it mean for alternative methane sensing technologies.* Petroleum Technology Alliance of Canada: Methane Emissions Reduction Forum, Banff, AB, Canada.

Karimi, F., & Karan, K. (2018, September 02-07) *Gas-fed CO_2 electrolysis in polymer electrolyte device.* International Society of Electrochemistry (ISE) Conference, Bologna, Italy.

Kazemi, N., Shor, R., & Innanen, K. (2018, June 11-14). *Seismic recording total least squares.* European Association of Geophysicists and Engineers (EAGE) Conference, Copenhagen, Denmark.

Lu., Q., & Song, P. (2018, October 28-31) *2D and 3D Metal-organic framework at the oil/water interface.* 68th Canadian Chemical Engineering Conference, Toronto, ON, Canada.

McKean, S. H., Priest, J. A., Eaton, D. W., Philips, J., & van der Baan, M. (2018, October 24-26). *An industry perspective on induced seismicity.* Banff International Induced Seismicity Workshop, Banff, AB, Canada.

Novotnik, B., Bryant, S., Larter, S., & Strous, M. (2018, Mar13-16). *Biological, metal dependent oxidation of hydrocarbons as a route to electricity generation.* The 13th Annual DOE Joint Genome Institute Genomics of Energy & Environment Meeting 2018, San Francisco, CA, United States.

Osadetz, K.G., Lawton, D.C, & Saeedfar, A. (2018, August 03-06). *No "Planet B": Are Gas Hydrates "The Clathrate Gun" at our Head or Part of the Solution?* MENSA Canada's 2018 Annual Gathering, Calgary, AB, Canada.

Paquette, A., Vadlamani, A., Demirkaya, C., Strous, M., & De la Hoz Siegler, H. (2018, October 28-31) *Reduce, Reuse and Recycle: The 3 R's of nutrient recovery for sustainable growth of microalgal biomass at high pH and alkalinity.* 68th Canadian Chemical Engineering Conference, Toronto, ON, Canada.

Radovic, J., Silva, R., Novotnik, B., Venkatesan, S., Thangadurai, V., Bryant, S., Strous, M., & Larter, S. (2018, July 29-August 3). *SYZYGY: Direct production of electricity from oil fields.* Gordon Research Conference in Organic Geochemistry, Holderness, NH, United States.

Singh, K., Kan, W. H., & Thangadurai, V. (2018, May 27-31). *Effect of the Ca/Nb ratio on the B-site ordering and electrical transport properties in double perovskite-type $Ba_3Ca_{1+x}Nb_{2-x}O_{9-\delta}$.* Canadian Society for Chemistry 101st Canadian Chemistry Conference and Exhibition, Edmonton, AB, Canada.

Singh, K., Oz, A., Gelman, D., Tsur, Y., & Thangadurai V. (2018). *Electrochemical properties of doped $Ba_{0.5}Sr_{0.5}Fe_{O3-\delta}$ cathodes.* Canadian Society for Chemistry 101st Canadian Chemistry Conference and Exhibition, Edmonton, AB, Canada.

Song, P., Natale, G., Wang, J., Bond, T., de la Hoz Sielger, H., Hejazi, H., Gates, I., & Lu, Q (2018, June 19-22) *Metal-organic framework at the oil/water interface.* 30th Canadian Materials Science Conference, Edmonton, AB, Canada.

Thangadurai,V. (2018, September 16-21) *Humidity and carbon dioxide stable solid state proton conductors derived from perovskite-type structure.* 19th International Conference on Solid State Protonic Conductors, Stowe, VT, United States.

Thorlakson, L., & Thomas, M. (2018, September 12-14) *Assessing political pathways for energy transition.* Global Climate Action Summit, San Francisco, CA, United States.

Utley, R., Gilfillan, S., Utting, N., Johnson, G., Haszeldine, S., Stuart, F., Osadetz, K., & Lawton, D. (2018, November 27-29). *Resolving the baseline isotopic fingerprints of Carbon Dioxide (CO_2) and Methane (CH_4) at the Carbon Management Canada Research Institutes Field Research Station, Canada.* Petroleum Exploration Society of Great Britain: PETEX 2018, London, United Kingdom.

Eaton, D. (2017, March 01-04). *Dynamics of fault activation by hydraulic fracturing in overpressured shale formations.* SEDHEAT Workshop, Salt Lake City, UT, United States.

Eaton, D. (2017, June 12-15). *Maximum magnitude and other conundrums of injection-induced seismicity.* 79th EAGE Conference & Exhibition 2017, Paris, France.

Oz, A., Gelman, D., Tsur, Y., Singh, K., & Thangadurai, V. (2017, July 23-28). *Evolutionary programming based approach for SOFC cathode characterization: A case study on Co — Co-free mixed conducting perovskites.* The 15th International Symposium on Solid Oxide Fuel Cells, Hollywood, FL, United States.

Ryan, M.C., Abboud, J.M., Law, A., & Lauer, R.M. (2017, June 26-28). *Towards a conceptual model for free phase gas transport in the subsurface.* International Association of Hydrogeologists Regional Flow Conference, Calgary, AB, Canada.

EXTERNAL AWARDS

First Name	Last Name	Agency	Prize/Award	Agency Type	Year Awarded	Status
Alexandre	Paquette	Canadian Society for Chemical Engineering	1st Place in the Graduate Energy Division Poster Competition	National	2018	Successful
Alexandre	Paquette	Canadian Society for Chemical Engineering	2nd Place in Overall Graduate Poster Competition	National	2018	Successful
Audrey	Laventure	NSERC	Postdoctoral Fellowship, NSERC 1st woman in Chemistry	National	2018 - 2020	Successful
Audrey	Laventure	UCalgary Faculty of Science	Innovation Postdoctoral Fellow	University	2019	Successful
Audrey	Laventure	NSERC	NSERC and L'Oréal-UNESCO For Women in Science Supplement	National	2018	Nominated
Audrey	Laventure	Canadian Society for Chemistry	Outstanding Poster Presentation	National	2020	Successful
Ehsan	Hosseini	UCalgary Graduate Students' Association	Graduate Student Sustainability-Honorable Mention	University	2019	Successful
Fatemeh (Parisa) Karimi	Amirkiasar	The International Society of Electrochemistry	Best poster award	International	2018	Successful
George	Ike	UCalgary Graduate Scholarship Committee	Eyes High International Doctoral Recruitment Scholarship ($15,000)	University	2020	Successful
Jean	Auriol	GdR Macs	French Ph.D. Award in Control by the GdR Macs (2018).	National	2018	Nominated
Jingyi (Jacky)	Wang	Oil and Gas Council WECA	Innovation of the Year Award	International	2019	Nominated
Joshua	Koenig	Queen Elizabeth Scholars	Queen Elizabeth II Scholarship	National	2018	Successful
Joshua	Koenig	Government of Alberta	Alberta Graduate Excellence Scholarship (AGES)	Provincial	2019	Successful
Marwa	Hannouf	FruiTrop Thema	Best Methodological SLCA Contribution	International	2020	Successful
Mozhou	Gao	PTAC	Winner of Student Led Poster Competition	National	2020	Successful
Nasser	Kazemi Nojadeh	Geoconvention	Best Oral Presentation	National	2019	Honourable Mention
Scott	McKean	Queen Elizabeth Scholars	Queen Elizabeth II Scholarship	National	2019	Successful
Shruti	Mendiratta	American Chemical Society	Best Oral Presentation	International	2019	Successful
Stuart	Burns	69th Annual Denver X-ray Conference (DXC2020)	Best poster award	International	2020	Successful
Zainab	Dadashi Forshomi	Chemical and Petroleum Engineering Graduate Students' Association (CPEG)	Best Presentation	University	2019	Successful

GLOSSARY OF ACRONYMS

AFM	Atomic force microscopy
AG	Silver
AQP	Catalytic aqua processing
ARMA	American Rock Mechanics Association
ATR	Autothermal reforming
Au	Gold
BAT	Best Available Technology
BDS	Biodesulfurization
BECCS	Bioenergy with carbon capture and storage
BET	Brunauer–Emmett–Teller
$Bi_2Sn_2O_6O'$	Bismuth pyrostannate
$BiVO_4$	Bismuth vanadate
BO-MD	Born-Oppenheimer molecular dynamic
C-1	One carbon
C_2H_2	Acetylene
CaMI	Containment and Monitoring Institute
$CaCO_3$	Calcium carbonate
CBM	Carbohydrate binding module
CCU	Carbon capture and utilization
CdS	Cadmium sulphide
CE	Canvas electrical grade
CF	Cellulose filament
CFD	Computational fluid dynamics
CFREF	Canada First Research Excellent Fund
CGI	Cyclic gas injection
CH_4	Methane
CIC	Colloid imprinted carbon
CLS	Canadian Light Source
CNC	Cellulose nanocrystals
CNC pincer	Carbon-nitrogen-carbon atoms of the ligand which bind the metal in the complex
CNF	Cellulose nanofibril
CNN	Convolutional neural network
CO	Carbon monoxide
CO_2	Carbon dioxide
CO_2RR	Electroreduction of CO_2
CO_3^{2-}	Carbonate ion
Cr	Chromium
CRM	Capacitance-resistance model
CSC	Catalytic steam cracking
cSOR	Cumulative steam-oil ratio
CuAAC	Copper(I)-catalyzed azide-alkyne cycloaddition
CV	Cyclic voltammetry
DAC	Direct air capture
DAS	Distributed acoustic sensing
DCSG	Direct contact steam generators
DFT	Density functional theory
DI	Deionized

DiD	Difference-in-differences
DPRIE	Downwind plume road intersection estimator
DRM	Dry reforming of methane
ED	Electrodialysis
EDS	Energy-dispersive X-ray spectroscopy
EGER	Enhanced geothermal energy recovery
EGR	Enhanced gas recovery
EIA	Energy Information Administration
EIS	Electrochemical impedance spectroscopy
EO	Ethylene oxide
EOR	Enhanced oil recovery
ERC	Electrochemical reduction of CO_2
ES-SAGD	Expanding solvent steam-assisted gravity drainage
EU ETS	European Union Emissions Trading System
EXAFS	Extended X-ray absorption fine structure
FCD	Flow control device
FEM	Finite element method
FRS	Field Research Site
FTE	Fundamental technology element
FTICRMS	Fourier-transform ion cyclotron resonance mass spectrometry
FTIR	Fourier-transform infrared spectroscopy
FWI	Full-waveform inversion
GC	Gas chromatographer
GHG	Greenhouse gas
GM	Gas migration
GNA	Gluconic acid
GPU	Graphics processing unit
GRA	Glucaric acid
GRI	Global Research Initiative in Sustainable Low Carbon Unconventional Resources
H_2S	Hydrogen sulphide
HaP	Hydroxyapatite
HMF	Hydroxymethylfurfural
HCOO-	Formate
HQP	Highly qualified personnel
HRDPS	High resolution deterministic prediction system
HTI	Horizontal transverse isotropic
HVSR	Horizontal-to-vertical spectral ratio
ICP	Ion concentration polarization
IFT	interfacial tension
IPN	Interpenetrating network
IPV	Indoor organic photovoltaic
ISUT	In situ upgrading technology
Kn	Knudsen number
kPa	kilopascal
LC	Liquid crystalline
LCA	Life cycle assessment
LCFCr	$La_{0.3}Ca_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$
LMFCr	$La_{0.3}M_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$
LSRTM	Least squares reverse time migration
MD	Molecular dynamics
MEM	Micro-electromechanical system
micro-PIV	Micro-particle-image-velocimetry
MOC	Molecular organometallic electrocatalyst
MOF	Metal-organic framework
MoS_2	Molybdenum disulfide
MSC	Modified Scheludko-cell
MSP	Minimum selling price
NCS	Nanoporous scaffold
NET	Negative emission technology
NFR	Naturally fractured reservoirs
NHC	N-heterocyclic carbene
Ni	Nickel
Ni-Mo	Nickel-Molybdenum
NiOx	Nickel (oxy)hydroxide
NIRDD	Near infrared driven decomposition
NMR	Nuclear magnetic resonance
NPV	Net present value
OER	Oxygen evolution reaction
OGCNN	Orbital graph convolutional neural network
OLEDs	organic light emitting diodes
OPV	Organic photovoltaics
ORT	Orthorhombic
OTSG	Once through steam generator
PCE	Power conversion efficiency
Pd	Palladium
PDI	Perylene diimide
PEG	Polyethylene glycol
Petcoke	Petroleum coke
PFPD	Post Fracture Pressure Decay
PLD	Pulsed laser deposition
PMOD	Photochemical metal-organic deposition
PNIPAm	Poly(N-isopropylacrylamide)
PO	Propylene oxide
POM	Polarization optical microscopy
PS	Passive seismic
Pt	Platinum
PTQ10	Red-coloured semiconducting polymer
PVT	Pressure volume temperature
PZT	Lead zirconate titanate
QLEDs	quantum dot LEDs
REB	Reverse emulsion breakers
ResNet	Residual neural network
RMS	Root mean square
RS-SAGD	Rich solvent steam-assisted gravity drainage
RTM	Reverse time migration
RuOx	Ruthenium oxide
SAGD	Steam-assisted gravity drainage
SAIT	Southern Alberta Institute of Technology
SAP	Solvent-aided process
SARA	Saturates, Asphaltenes, Resins and Aromatics Analysis
SCVF	Surface casing vent flows
SDE	Stimulation distribution effectiveness
SDS	Sodium dodecyl sulfate
SEM	Scanning electron microscope
SEV	Sensor equipped vehicle
SGER	Alberta Specified Gas Emitters Regulation
SHE	standard hydrogen electrode
SLS	Standard linear solid

SMR	Steam methane reforming
SO_3H	Sulphonic acid
SOEC	Solid oxide electrolysis cell
SOFC	Solid oxide fuel cell
SOR	Steam-to-oil ratio
SPE	Society of Petroleum Engineers
SWD	Seismic-while-drilling
TAPPy	1,3,5-triazapentadienyl-2,4-bis(2-pyridyl)
TEA	Techno-economic analysis
TEM	Transmission electron microscopy
TGA	Thermogravimetric analysis
TG-DTA	Thermogravimetry-differential thermal analysis
THAI	Toe-to-heel air injection
TI	Transverse isotropy
TLF	Thin liquid film
TML	Technology markup language
TOF	Turn over frequency
TTI	Tilted transverse isotropic
U	electric potential vs. SHE
UAOD	Ultrasound-assisted oxidative desulphurization
UGF	Unified gas flow
U-net	A Fully Convolutional Network (FCN) that does image segmentation.
UV-Vis	Ultraviolet-visible spectroscopy
VASP	Vienna ab initio Simulation Package
VSP	Vertical seismic profile
VTI	Vertical transverse isotropic
WAG	Water alternating gas
WLS	warm lime softening
WTW	Well-to-wheel
W/O	Water/oil
XRD	X-ray diffraction
XPS	X-ray photoelectron spectroscopy
ZIF	Zeolitic imidazolate frameworks
ZP	Zeta-potential
2D	two-dimensional
2D-GO	Two-dimensional graphene oxide
3D	three-dimensional