UNIVERSITY OF CALGARY

THE GLOBAL RESEARCH INITIATIVE:

FUELING A CLEAN ENERGY FUTURE

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THE GLOBAL RESEARCH INITIATIVE:

FUELING A CLEAN ENERGY FUTURE

Attention: Global Research Initiative — Research Publication
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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.

This research has been conducted, in part, thanks to the **Canada First Research Excellence Fund**.

FOREWORD

When the Government of Canada announced the new Canada First Research Excellence Fund (CFREF) in 2014, the University of Calgary was already deeply engaged in a multi-disciplinary effort to reduce the carbon footprint of energy development. Our research strategy — *Energy Innovations for Today and Tomorrow* identified major challenges and brought together our faculty members to work on solutions. The CFREF program was heralded as a move towards global excellence and partnerships, attracting and retaining global talent to Canadian universities and expanding the commercialization of research findings.

At the time, I was serving as the Vice-President (Research) and we immediately saw this as an ideal opportunity for our scholars to demonstrate their international leadership in clean technologies. Our team mobilized clean energy expertise from across campus, drawing from a wide range of disciplines in engineering, biological sciences, geoscience, chemistry, geology, health sciences and public policy. Together with the Southern Alberta Institute of Technology (SAIT) and its energy specialists, the University of Calgary carefully assembled an ambitious multidisciplinary research submission for CFREF: the Global Research Initiative in Sustainable Low Carbon Unconventional Resources (GRI).

Our joint submission for the CFREF program outlined several large-scale initiatives designed to address all aspects of a low-carbon energy future. GRI acknowledges the increasingly urgent issue of climate change, fostering mutually beneficial partnerships with industry to produce carbon-neutral energy systems and renewable energy via solar and wind power.

The GRI team reflects the expertise of over 270 researchers and outlines three broad themes of research: heavy oil and bitumen, tight oil and gas, CO_2 conversion, and a cross-cutting platform of technology assessment. Guided by our theme leads and our highly qualified personnel (HQP), these themes encompassed grand challenges aimed at:

- reducing viscosity of heavy oil and bitumen at moderate temperatures;
- imaging and controlling *in situ* flow processes;
- imaging and controlling hydraulic fracturing, enabling small-footprint recovery from low-permeability reservoirs;
- reducing CO_2 emissions to zero at petroleum reservoirs;
- and optimizing CO_2 capture and conversion catalysis.

In 2016, the University of Calgary-SAIT joint submission was approved by the Canada First Research Excellence Fund and awarded $75 million to realize this ambition of a clean energy future.

Over the past two years, the GRI team, the theme leads and the HQP have marshalled their assembled expertise to make real advancements in Canada's ability to reduce the carbon footprint of resource development, establish clean technologies for unconventional oil recovery, store and convert CO_2 from industrial applications, and promote solar, wind and CO_2 power generation. Our campus community is incredibly proud to host this significant research enterprise in support of Canada's health, environment and economy — now and well into the years ahead. We are fortunate to have government and industry partners around the world, translating our energy research into real-world solutions.

This publication details the ingenuity and determination of an extraordinary team of multidisciplinary researchers, collectively working towards clean energy and results that will benefit Canadians for generations to come. Canada is ready for the future of clean energy technologies, and UCalgary is ready to shine a light on our GRI team making this a reality.

Edward McCauley, PhD, FRSC
President and Vice-Chancellor

In 2016 when the University of Calgary, in partnership with SAIT, was awarded $75 million from the Canada First Research Excellence Fund, I knew this was an incredible opportunity for our institution to transform energy research. We quickly launched the Global Research Initiative in Sustainable Low Carbon Unconventional Resources (GRI) and in many ways, this endeavor is one of the biggest undertakings in our institution's history.

The research being conducted within the GRI is the result of a multidisciplinary, cross-campus effort that has provided a unique opportunity for our institution. We are developing solutions for some of the greatest challenges facing the global energy industry and pressing issues confronting the environment.

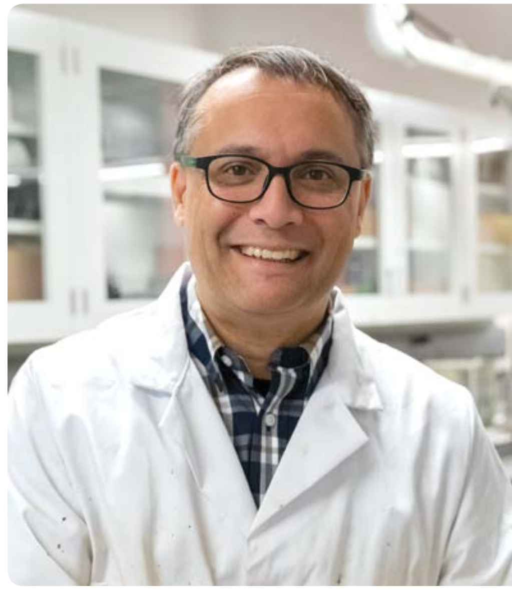
The purpose of this book is to develop a record of the GRI's tremendous efforts in energy research, to celebrate our achievements and milestones, and to shine a spotlight on the hard-working individuals who are the cornerstone of our research activities.

A key ingredient to achieving our goals are the highly qualified personnel (HQP) — the students and post-doctoral scholars — who are the lifeblood of these research projects. Their ideas, enthusiasm and passion drive much of what we do as a research-intensive university. Their energy and tireless pursuit of excellence enables us to deliver on our commitment to take our energy research from great to best, to operate 'not business as usual', and to make significant impacts in scholarship, training, industry solutions, and contributions to the community.

The University of Calgary has both the opportunity and responsibility to be a global leader in high-impact energy research. I continue to be amazed at what we are achieving in the lab and when we bring our technology and concepts to our end-users. We have come a long way in a short period of time and I am very excited to see what our researchers will accomplish in the GRI program.

Enjoy this record of our achievements!

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



"We are developing solutions for some of the greatest challenges facing the global energy industry and pressing issues confronting the environment."

CONTENTS

THEME 1: HEAVY OIL & BITUMEN

Unconventional petroleum resources are typically defined by being of low mobility — either high viscosity oil (e.g. heavy oil or bitumen) or low permeability reservoir rock (e.g. tight oil and gas, shale). The focus in Theme 1, is on systems containing high viscosity heavy oil and bitumen. Typically, heavy oil has viscosities between thousands and a few tens of thousands of centipoise (unit of dynamic viscosity) whereas bitumen has viscosities exceeding one hundred thousand centipoise and often in the millions of centipoise.

There are two requirements that must be met to produce these resources — first, mobilize the oil (lower its viscosity) and second, move the mobilized oil to a production well. At present, for oil sands reservoirs, bitumen mobility is improved by injecting high temperature and pressure steam into the reservoir. This implies high cost and greenhouse gas emissions from these recovery processes.

Research in Theme 1 is focused on improving oil mobility and imaging, and controlling the recovery processes to lower the environmental impact, improve the economics and raise the energy efficiency of these processes. Theme 1 specific targets of the research being conducted are the use of additives with mild heating to improve bitumen mobilization as well as next generation drilling, monitoring and control to improve recovery process performance.

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. Jalel Azaiez, Steve Larter, Brij Maini, Joule Bergerson, Hossein Hejazi, Stephen M. Hubbard, Kristopher Innanen, Qingye (Gemma) Lu, Giovanniantonio Natale, Roman Shor and Hector De la Hoz Siegler.

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, Giovanniantonio Natale, Qingye (Gemma) Lu, Hector De la Hoz Siegler

Background

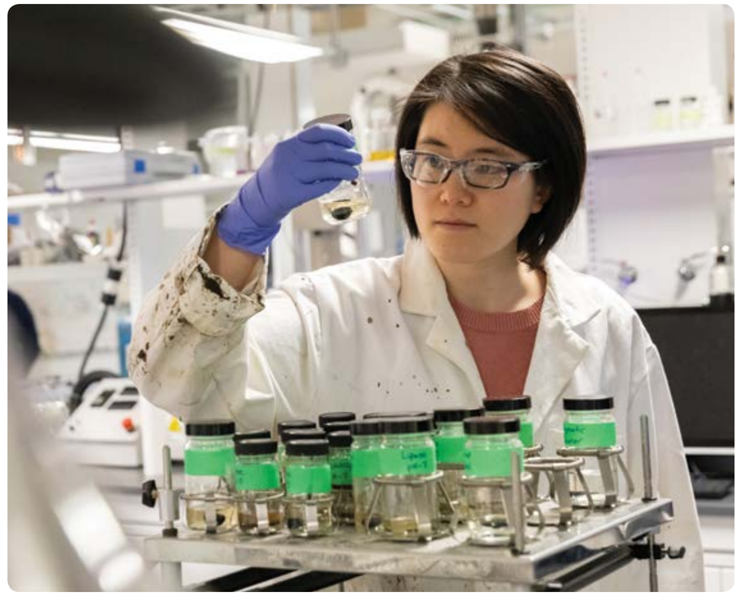
At present, steam-based recovery processes for oil sands reservoirs are both energy and greenhouse gas (GHG) emissions intensive relative to other petroleum production processes. The key reason for the use of steam is that it is an excellent carrier of sensible and latent heat which raises the temperature 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 microparticles and how they behave at interfaces. Furthermore, research on modelling the behavior of nano and microparticles 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

Md. Mohosin Rana
PhD student

Introduction

Climate change and increased global energy demand requires a dramatic reduction in the greenhouse gas (GHG) emissions associated with fossil fuel production. Additives (e.g. surfactants, catalysts, solvents) can be used to improve the energy efficiency of crude oil recovery operations, mitigating GHG emissions and making them more environmentally friendly. Md. Mohosin Rana works on 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. The challenge is to design a carrier capable of withstanding reservoir conditions and that can be effectively delivered into the formation.

Results

Initially, the research team focused on the tuning of the lower critical solution temperature (LCST) range of poly(N-isopropylacrylamide) (PNIPAm) polymers by synthesizing them in different solvent mixtures (dioxane, tetrahydrofuran, toluene, etc.). So far, hydrogel synthesized in dioxane solvent showed the better LCST response (hydrophobicity at 41 C; hydrophilicity at 21 C) (see Figure 1). The research team plans to tune the molecular weight of the polymer by changing cross-linking density. Increasing the mechanical stability of PNIPAm polymer to work in harsh reservoir environments is another major aim of this research. To achieve this, the team is trying to develop the interpenetrating network (IPN) of PNIPAm in combination with cellulose (obtained from algal source). In future work, the team will check multiple synthesis protocols to reach the target hydrogel size at the nano-scale. Finally, they are designing a small-scale encapsulation device for the highly efficient encapsulation of additive molecule inside the hydrogel.

Conclusions

So far, polymer hydrogel synthesized in dioxane has better LCST response than other solvents.

IPN of PNIPAm-based hydrogel would be a better choice in terms of mechanically strong hydrogel performance.

Small-scale polymer hydrogel-based smart-carrier should be a useful option for more cost-efficient and effective heavy oil recovery.

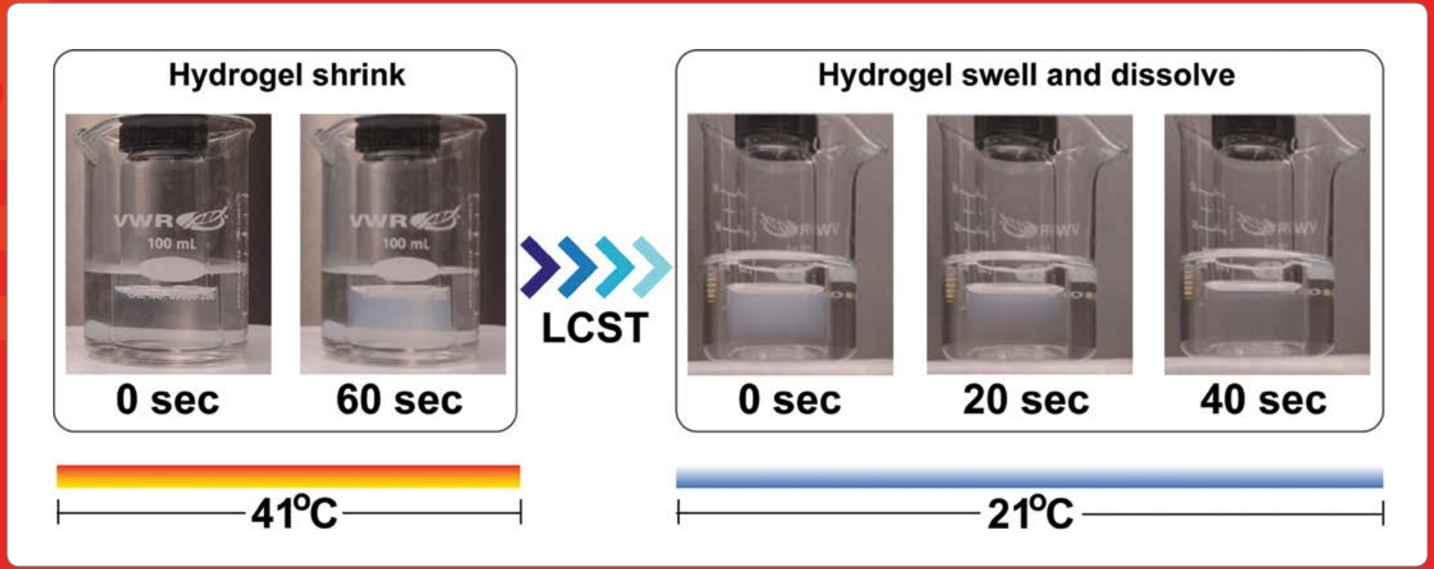
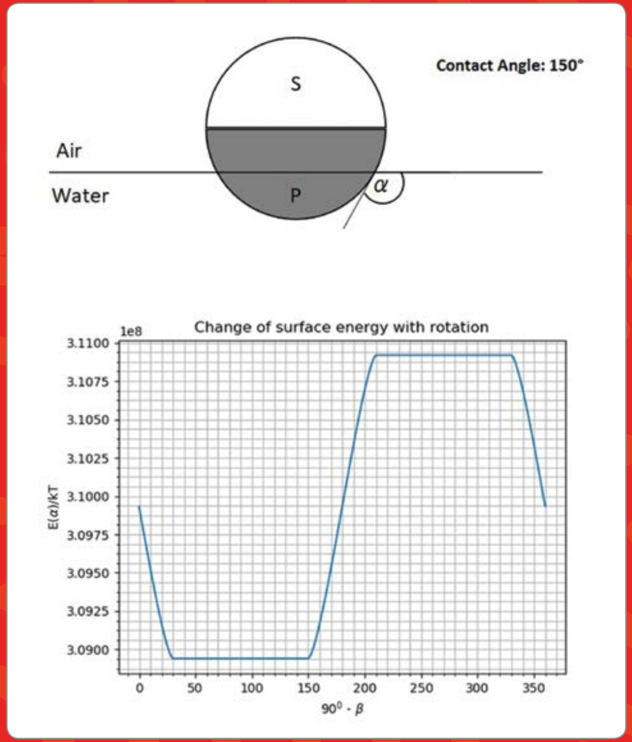
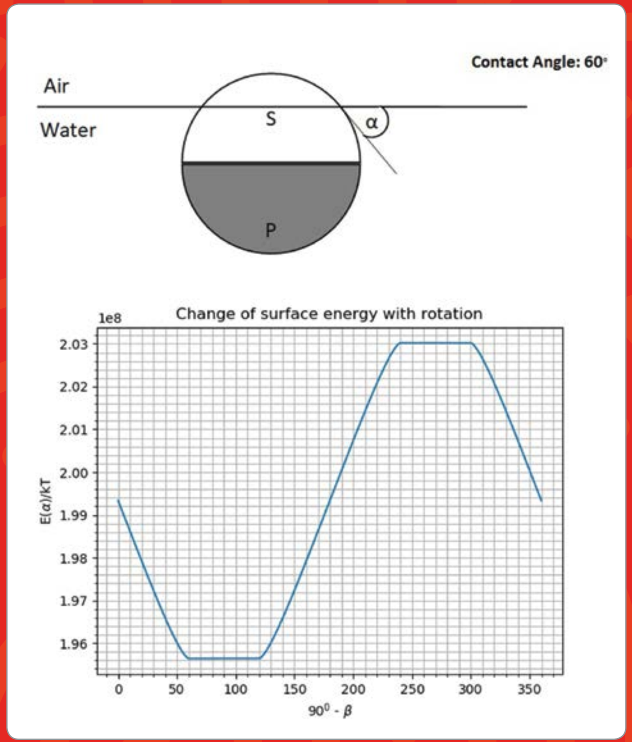


Figure 1: **Low Critical Solution Temperature (LCST) behavior of PNIPAm hydrogel at different temperature.** At high temperature they started to shrink and form thick gel, while at low temperature they started to swell and dissolve in the solution.





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

Mohammad Tanvir Hossain
PhD student

Introduction

This project aims to understand the behavior 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, 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 behavior 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 of an amphiphilic Janus sphere then extending it to rotational motion of the Janus sphere at interface. Later a more general theoretical framework for the motion of a Janus sphere have developed that coupled the translation and rotation of the particle. One of the major challenges that the research team overcame was derivation of surface energy of the particle at the interface that change with the orientation of the particle itself. On the numerical side, the team developed an algorithm to solve the coupled Langevin equations (position and rotation). These two stochastic differential equations are coupled via the surface energy and the hydrodynamic drag.

Conclusions

The team developed a theoretical framework to describe the behavior of a single amphiphilic Janus particle.

A range of physical conditions showed that the particle continuously rotates at the interfaces. This result motivates the possible applications to enhance mass, heat and moment transfer at interfaces.

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

Ping Song
Postdoctoral Fellow

Introduction

Dr. Ping Song, PhD, works on the investigation of metal-organic frameworks (MOFs) at the oil/water interfaces. The challenges are synthesis of the optimized nano-MOFs and characterization methods of their interfacial behaviors. The aims of this project are to characterize the interfacial behavior of a number of representative MOFs and find out the mechanism of stabilization at the interfaces. This work provides great insights in further application of MOFs in oil recovery as well as the development of novel composites and membranes.

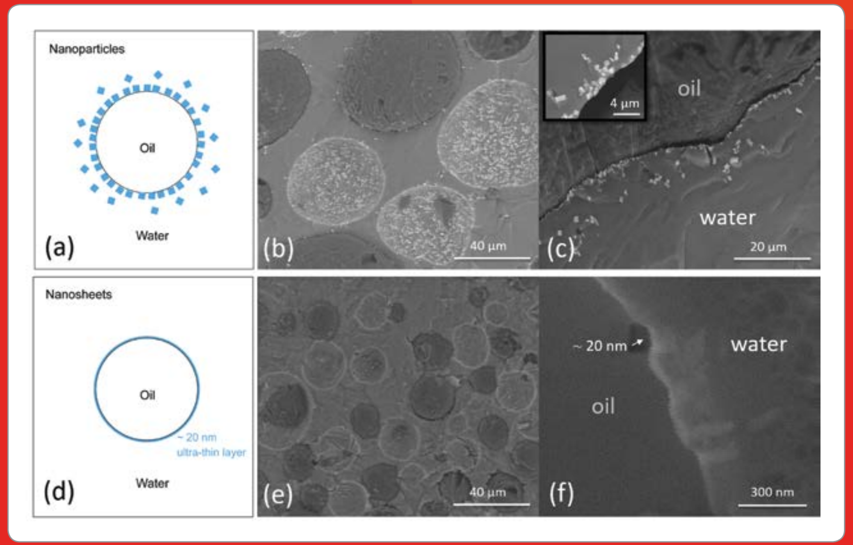
Results

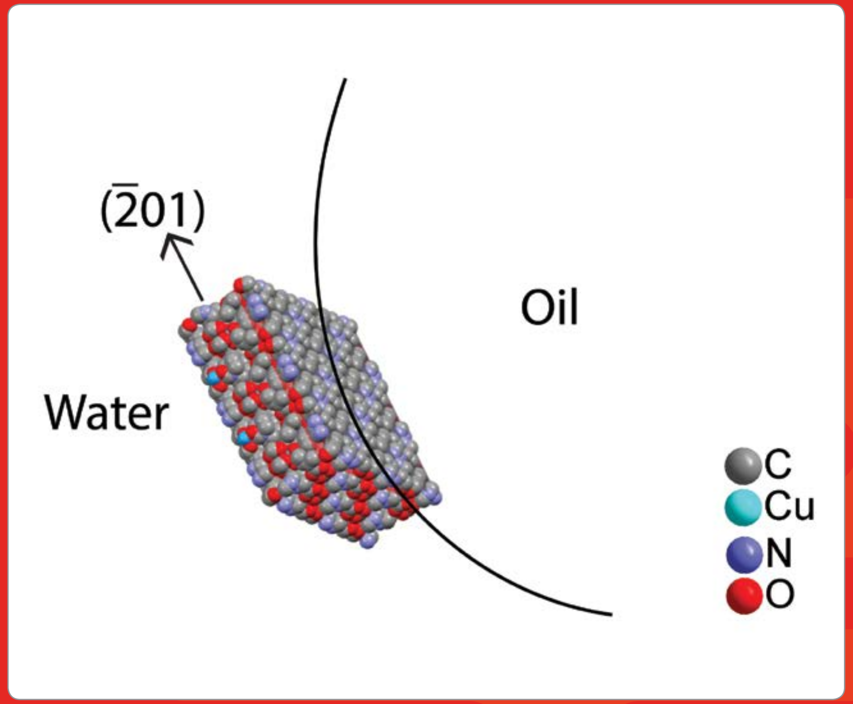
The interfacial behavior of two-dimensional (2D) MOFs has been investigated. In this work, the distribution and partition of 2D nanosheets (NS) and three-dimensional (3D) nanoparticles (NP) of copper benzenedicarboxylate (CuBDC) at the oil/water interface are imaged by cryo-SEM. A layer of approximately 20 nanometers NS-CuBDC is detected along the interface. The hydrophilic CuBDC localizes along the interface within the water phase. The exchange of water into the CuBDC structure leads to super hydrophilic wettability. Due to the amphiphilic properties, NP-CuBDC is used as sole stabilizer to form stable oil-in-water emulsions. Synchrotron-based computed tomography was used to image the 3D distribution of CuBDC in emulsions at room temperature. This work has provided great insights in the fundamental study of MOFs at the oil/water interface and further development of ultra-thin 2D MOF membranes.

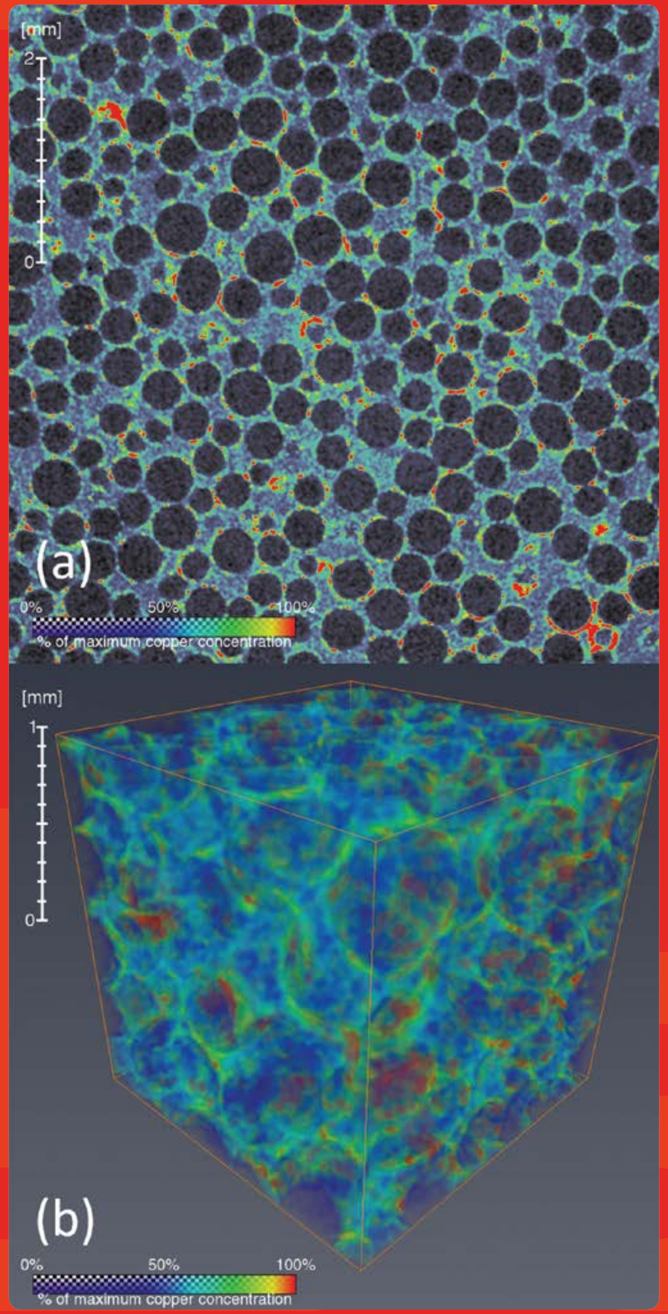
Conclusions

- CuBDC nanosheets and nanoparticles were found to form a layer along the oil/water interface and within the water phase.
- CuBDC nanoparticles were demonstrated as sole stabilizer in the formation of stable Pickering emulsions.
- This work provided great insights in understanding the interfacial behavior of 2D and 3D MOF materials.

Dr. Ping Song acknowledges the technical support received from Canadian Light Source.







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

Ranjani Kannaiyan
Postdoctoral Fellow

Introduction

Bitumen undergoes structural and compositional changes throughout the process of recovery, separation and transportation caused by various factors such as pressure, temperature and shear. What happens to the long chain of low and high molecular weight hydrocarbons and how it affects the rheology will help to shed light on improving the processes by using appropriate solvents and controlling the shear. The main focus of the project is to understand the molecular behavior of bitumen in the presence of solvents and asphaltenes, and establish a relationship between the rheological properties and molecular arrangement in bitumen.

Results

Asphaltenes are nanoscale in bitumen and these molecules are dispersed in the maltene solvent. The addition of five per cent of heptane to bitumen results in desorption of a very small portion of resins and the nanoaggregates of asphaltenes are slightly in large scale but dispersed far from each other. Increasing the asphaltene content of bitumen by six per cent results in crowding of maltenes with asphaltenes and hence more resistance to flow. Mechanical rigidity of bitumen is proportional to the asphaltene content. Bitumen is composed of multiple phases, and the maltene and asphaltene phases are distinguishable at 25 C [atomic force microscopy (AFM) images]. However, from the Han plots, phase separation is observed around 40 C. Five per cent heptane in bitumen causes phase separation at 20 C, which is due to the increased distance between the moieties in the presence of heptane. Atomic Force Microscopy images of bitumen with additives support the existence of microstructure of the moieties in bitumen.

Conclusions

The effect of temperature on the viscosity behavior of bitumen with and without heptane and asphaltenes followed the Arrhenius model.

Asphaltenes govern the elastic part of the viscoelastic nature of bitumen and the higher the asphaltene content, the higher the effect of frequency on complex viscosity.

At temperatures 40 C and above, thermal effect predominates the molecular motion of molecules rather than angular frequency/shear effect.

Multiple phases in bitumen coexist as a single phase at normal conditions and become immiscible at 40 C.

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

Serena (Yixiao) Liu
MSc student

Introduction

As part of the Beyond Steam project, the research team is examining new materials in the form of nanoparticles that can be active at oil-water interfaces to improve the displacement and recovery of oil. The team conducted experiments in sand packs by using metallic organic framework (MOF) nanoparticles at the Canada Light Source, and is now examining the impact of these nanoparticles on larger scale interfacial effects by using a Hele-Shaw device. They will study interface shape, complexity, flow patterns and oil recovery in the Hele-Shaw cell by using MOFs suspended in the water phase.

Results

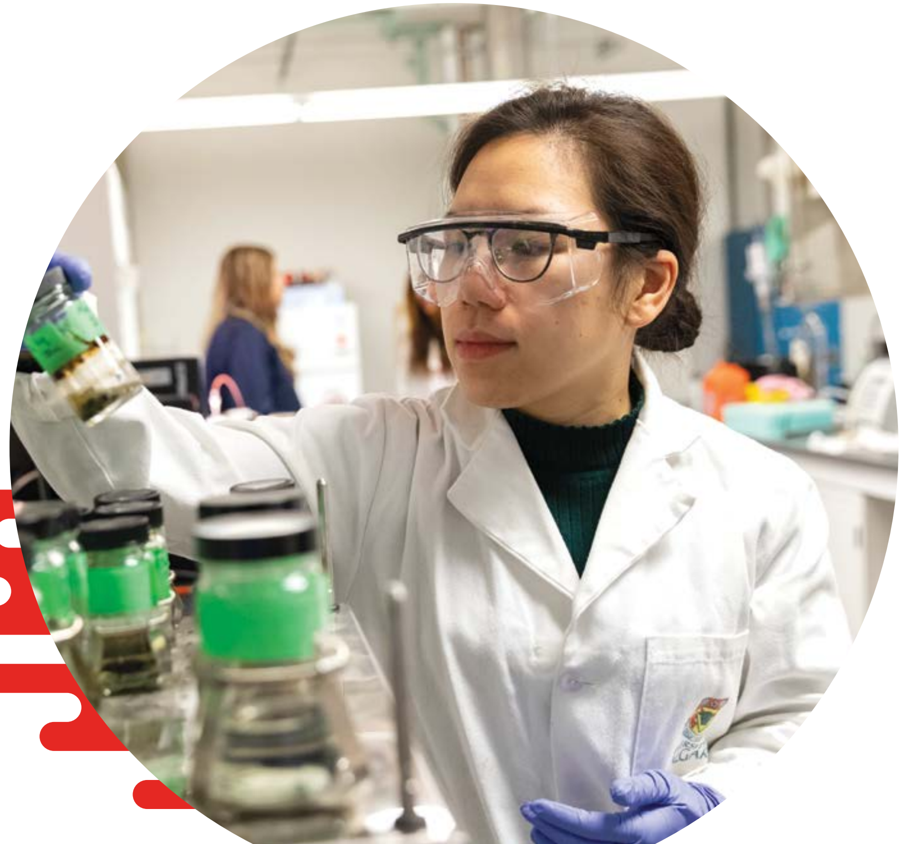
The Hele-Shaw apparatus has been designed, constructed and has been tested. Various shim materials have been tested and the gap the team has chosen for experiments is 0.015 inches (381 microns). Flow tests with water have been conducted to ensure that the apparatus does not leak and that the data acquisition system is functional — this includes the pressure transducers, flow rate, image capture and image analysis. The next step is to initially fill the Hele-Shaw cell with the chosen oil and then flood the system with the MOF suspensions of different concentrations.

Conclusions

Metallic organic frameworks (copper, zinc based) have shown promise for interfacial activity for oil-water systems.

Hele-Shaw apparatus is constructed, has been tested, and will be ready for viscous oil displacement tests in early 2019.

Effect of concentration and type of nanoparticle will be tested for its impact on interfacial shape and complexity in the Hele-Shaw cell.

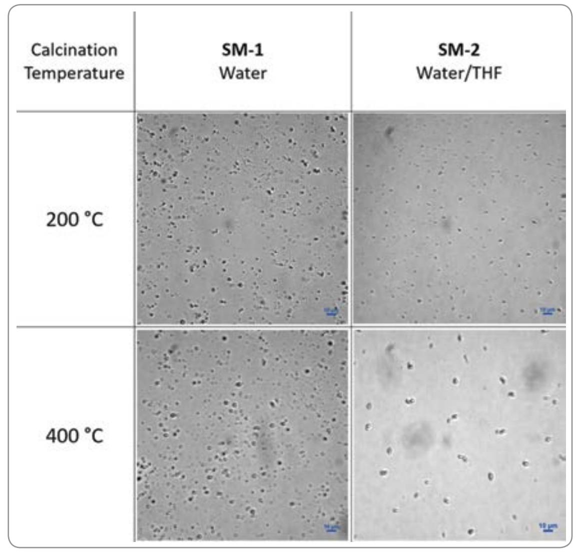


Beyond steam — additives to significantly improve the emissions and energy intensities of oil sands recovery processes

Shruti Mendiratta
Postdoctoral Associate

Introduction

Hydroxyapatite (HaP) is a well-known calcium phosphate-based ceramic that plays an important role in bioengineering and materials science. Its activity at the oil-water interface has not been extensively explored. The plethora of shapes and morphology of HaP particles motivates the research team to synthesize them and use them as a foundation for developing functional particles (core-shell, hollow, stimuli responsive and Janus) that can arrange themselves at oil-water interfaces or alter the wettability of rock surfaces. Viscous oil mobilization using HaP particles is one of the desired outcomes of this project.



Results

Dr. Shruti Mendiratta, PhD, has synthesized hydroxyapatite nanoparticles using two kinds of solvent systems: water-based and water-tetrahydrofuran-based. Fourier-transform infrared spectroscopy (FTIR) and powder X-ray diffraction (XRD) analyses revealed that the particles were pure and their peaks matched well with the simulated patterns. The particle size, charge and morphology of these particles will soon be investigated using various physical and imaging techniques. The research team wishes to investigate the synthetic methods and reaction parameters to regulate the particle shape and size.

The team will test the arrangement and influence of HaP on the evolution of oil-water interfaces using confocal laser scanning microscope and micro-particle image velocimetry. Judicious surface modification of these particles by conjugation or grafting to various kinds of molecules may enable flow manipulation.

Conclusions

Hydroxyapatite particles are promising foundation materials for synthesizing functional particles (core-shell, hollow, stimuli responsive and Janus).

An account of tailor-made HaP particles for viscous oil mobilization and their visualization through new imaging techniques may improve the understanding of the role of nanoparticles on fluid flow and their arrangement and interactions present at oil-water interfaces.

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

Xuemin Huang
PhD student

Introduction

The intent of this research project is to examine the wettability of hydrophilic and hydrophobic roughened surfaces in water-air and water-oil systems. There are many factors affecting the description of the wettability, such as surface energy, contact angle, surface composition and surface roughness. The scale of the roughness and its impact on the apparent contact angle will be studied. The research team will also examine surfaces with mixed wettability where some fraction of the roughened surface is water-wet and the rest of it is not. The goal is to develop a new theory describing wetting phenomenon more comprehensively.

Results

A repeatable procedure has been established to construct hydrophilic, hydrophobic and mixed wettability rough surfaces.
An apparatus has been constructed to visualize droplets on the roughened surfaces. The results for a water-air system show that the apparent contact angle is hard to define for rough surfaces since it varies around the three-phase contact line. An analysis of the images reveals the complexity of the wetting line on the roughened surface and the surface energy. A new thin film analyzer has permitted a detailed examination of the roughness of the surfaces to further quantify and characterize the surfaces. On mixed wettability surfaces, the water drop can be stable or collapse depending on the content of the water-wet grains.

Conclusions

Depending on the amount of hydrophilic grains, a water drop on a mixed wettability surface may be stable or collapse.

Surface roughness and wettability heterogeneity greatly impact the wetting process on roughened surfaces and the apparent contact angle.

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

Bitumen biodegradation by commercial hydrolytic enzymes

Michael Mislan
PhD student

Introduction

The project aims to enable the next generation of bitumen bioremediation, bioupgrading and bioprocessing by finding hydrolytic enzymes able to break down organic components of bitumen. The process is based on a novel paradigm of deposition and diagenesis which reconceptualizes bitumen as a geochemically fossilized form of soil. By partially breaking down bitumen to release sugars, fatty acids and other biochemical building blocks it is possible to provide readily bioavailable nutrient sources for microbial communities during remediation, further process these biochemicals into value-added products, or otherwise support biocompatible development of heavy oil resources after they become abandoned leases.

Results

The main outcome from the research so far has been the creation of a new, foundational tool for petroleum microbiologists and bioengineers to create novel bioprocesses, methods and metabolic pathways built on common biochemical inputs that can now be sourced directly from bituminous resources. By understanding the compositional and structural evolution of humic organic matter from the original ecosystem dynamics, which formed the soil through maturation, maltenic and asphaltenic moieties derived from some of the main biochemical building blocks of life such as sugars and fatty acids, were identified and released by aerobic fermentation with two of the most abundantly produced enzymes available in the existing market. While not demonstrating a significant improvement in bitumen viscosity or asphaltene degradation as originally sought, preliminary tests with oil sand have demonstrated an improvement in bitumen mobilization.

Conclusions

Bitumen can be partially broken down by two common, commercial hydrolytic enzymes to release sugars and fatty acids respectively.

Enzymatic-based recovery processes may have potential for producing oil sands at lower energy intensities than that of steam-based processes.

Michael Mislan acknowledges the Computer Modelling Group for use of STARS™.

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

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

Samaneh Ashoori
PhD student

Introduction

The intent of the project is to design a new, less emissive process of oil sands bitumen 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 remain unclear. Mineral dissolution/precipitations as a result of supercritical CO_2 injection in sandstones containing bitumen, along with aquathermolysis and steam-rock reactions are studied. There is potential that some fraction of the CO_2 injected will be stored in the reservoir and thus will not be emitted to surface. The research will provide directions for the design of DCSG-based SAGD recovery processes where the CO_2 emission intensity is reduced.

Results

Main outcomes from the research so far include qualitative identification of CO_2 trapping under mineral reactions in Athabasca sandstones. The team uses PHREEQC, a geochemical reaction code used to model equilibrium and kinetic geochemical reactions under CO_2 injection. The ultimate fate of CO_2 in the reservoir will be predicted by integrating the geochemical reactions into a SAGD thermal reservoir simulation model. Results so far suggest that the balance of carbonate minerals dissolution and precipitation rate is in favor of CO_2 trapping especially in forms of dolomite and dawsonite. The literature review indicates that sandstones are more suitable candidates for CO_2 storage over carbonates. CO_2 injection in carbonates lower the pH resulting in carbonate dissolution. Whereas the dissolution of aluminosilicates in sandstones buffers the pH and provides cations to react with bicarbonate ions (product of CO_2 dissolution in formation water) resulting in precipitation of carbonate mineral and thus permanent CO_2 trapping.

Conclusions

Geochemical modelling of Athabasca oil sands formation water and mineral composition reveals the fate of co-injected CO_2 in the reservoir during SAGD.

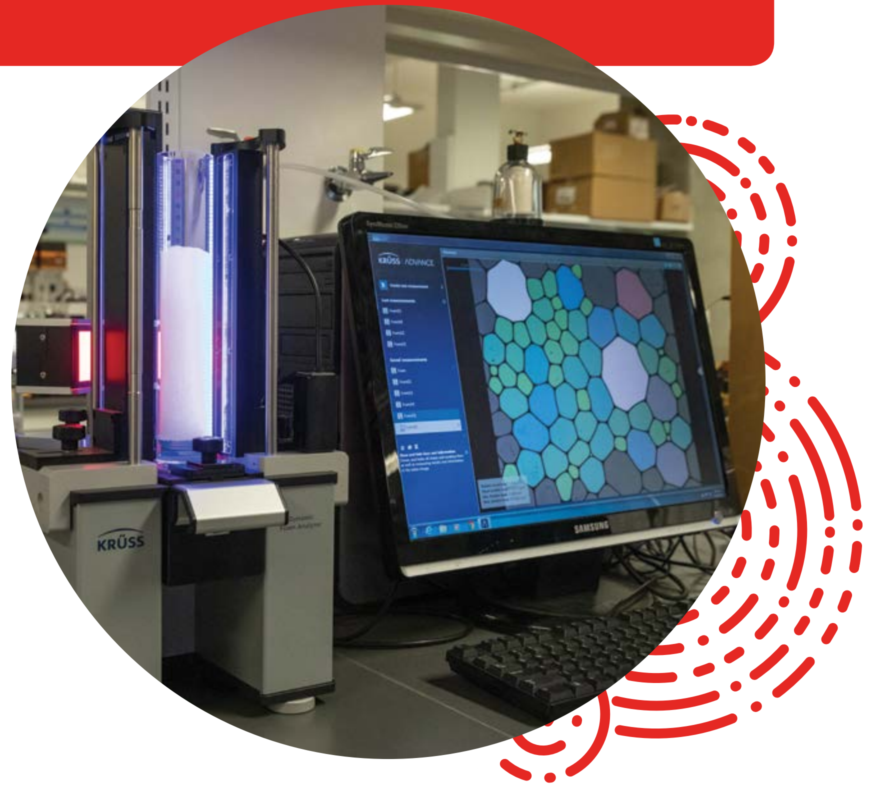
SAGD modelling with geochemical reactions for CO_2 and aquathermolysis is complex with long run times.

Given the finite size of SAGD chambers, storage of CO_2 will not be large if in the gas phase.

Samaneh Ashoori acknowledges the Computer Modelling Group for use of STARS™ and Schlumberger for use of Petrel and Eclipse.

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

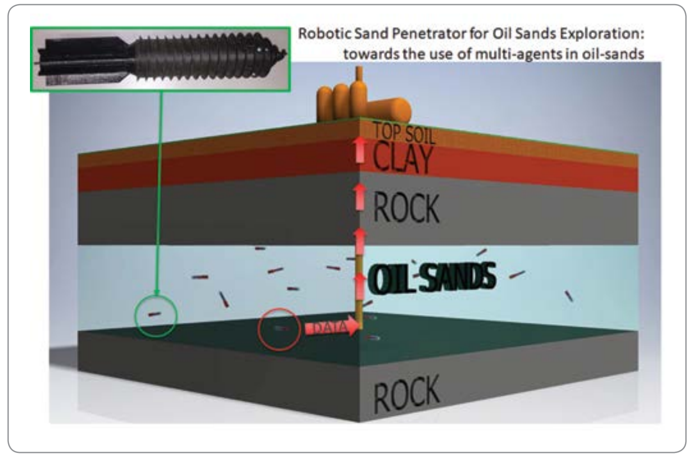
This project will present a new workflow to collect and analyze seismic-while-drilling data, develop and deploy new real-time drill string dynamics models suitable for real-time control, propose new well plans and wellbore completions for improved steam conformance, and develop a framework (and prototype) 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.

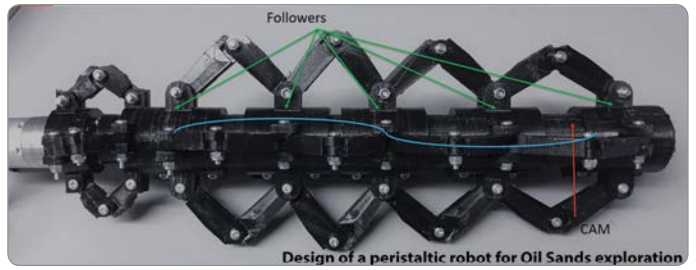
Next-generation adaptive wells and optimal placement for improved recovery

Juan Oziel De la Fuente Valadez
Postdoctoral Fellow

Introduction

This research is a collection of four projects creating opportunities to improve understanding of oil sands, and create more efficient and accurate processes. In the first project, Dr. Juan Valadex, PhD, aims to develop new technology to explore oil sands with a network of autonomous robots. The goal of this project is to build a group of robots that can collect data from oil sands and take tools to the reservoir in an autonomous manner. Juan also aims to design and build a drill string whirl machine that emulates the mechanical behavior of a real drill string. This will provide a method to get accurate representation of the mechanical characteristics of a real drill string in a laboratory setup. Juan is also working on an engineering design competition for high school students, to design a device that can penetrate non-consolidated media and give them an opportunity to learn about the oil sands and the challenges involved in oil production. And lastly, Juan is working on a project focused on carbon capture using the mallard reaction. This project will process biomass capture carbon from the atmosphere for storage.





Results

The research team is developing prototypes of the autonomous robots for oil sands exploration. The drill string whirl machine is being built and should be ready for testing in early 2019. This tool will be able to test control algorithms for drill string in the laboratory. The student engineering design competition will create a way to reach out to the local community and increase understanding of the oil sands, and challenges faced by those working in oil production. The carbon capture project will investigate another method of carbon capture and storage.

Conclusions

Autonomous robots designed to explore oil sands will improve the mapping of the reservoir and the effectiveness of the production.

A drill string whirl machine that emulates the mechanical behavior of a real drill string will provide opportunities to test control algorithms.

Next-generation adaptive wells and optimal placement for improved recovery

Nasser Kazemi Nojadeh
Postdoctoral Fellow

Introduction

Dr. Nasser Kazemi Nojadeh, PhD, aims to integrate seismic and seismic-while-drilling (SWD) data with development and production workflows to increase the productivity of the oil reservoirs, and reduce the uncertainties of well-placement and the prediction of future production. This is accomplished by providing accurate and high-resolution subsurface images. To do so, Nasser uses drill bit-rock interaction as a seismic source to image the subsurface with reduced uncertainties. This technology, called SWD imaging, results in better well placement and increased productivity. The research team is in the process of filing a patent for this technology. Nasser is also working on a reservoir characterization project that introduces a unique sampling methodology to improve the history matching and prediction of static and dynamic production data. This technology will help the team to increase production by improving the production plan.

Results

First, Nasser showed that subsurface imaging using SWD dataset is possible. The results of this research have been published. Figure 1 shows a SWD acquisition and Figure 2 shows the subsurface image derived from SWD data. To validate the results, the team is building, in collaboration with the University of Calgary's geoscience department, a physical model to acquire a realistic benchmark dataset for this technology. Second, Nasser developed a unique algorithm to improve the resolution of subsurface images, also published. Figure 3A shows the final subsurface image acquired using conventional seismic imaging and Figure 3B depicts the results of a new high-resolution technique. Finally, the research team is introducing a unique sampling methodology to better characterize the subsurface permeability field and improve production. The proposal of this technology is accepted for presentation, and the team is in the process of writing a full paper for this methodology.

Conclusions

- Integrating seismic and SWD with well-placement workflow increases oil production.
- SWD technology reduces the uncertainties of well-placement by providing high-resolution subsurface images.
- Integrating seismic data with reservoir characterization improves the predictability of production and results in the improved future production plan.
- Seismic data provides an opportunity to build a physically plausible and more realistic subsurface model that honors the geology.

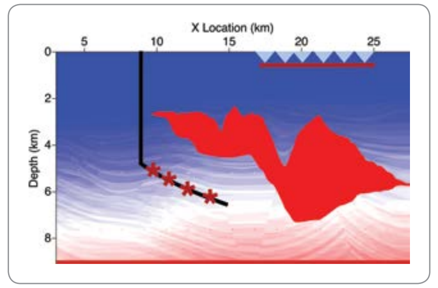


Figure 1

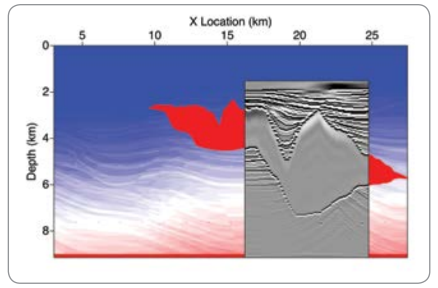


Figure 2

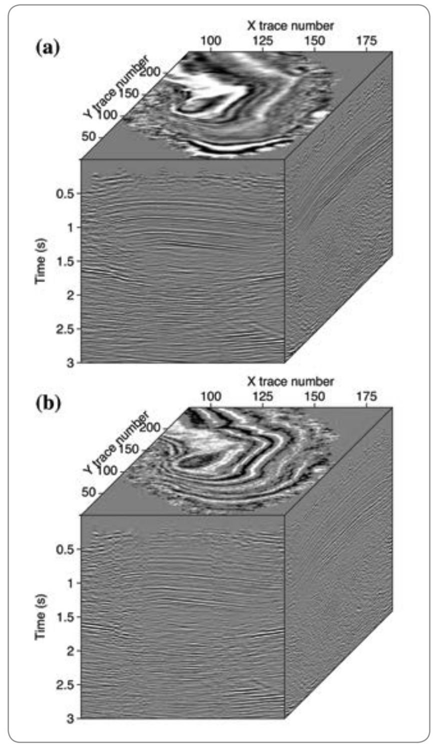


Figure 3

THERMAL SOLVENTS FOR *IN SITU* PHASE SEPARATION

Brij Maini

Background

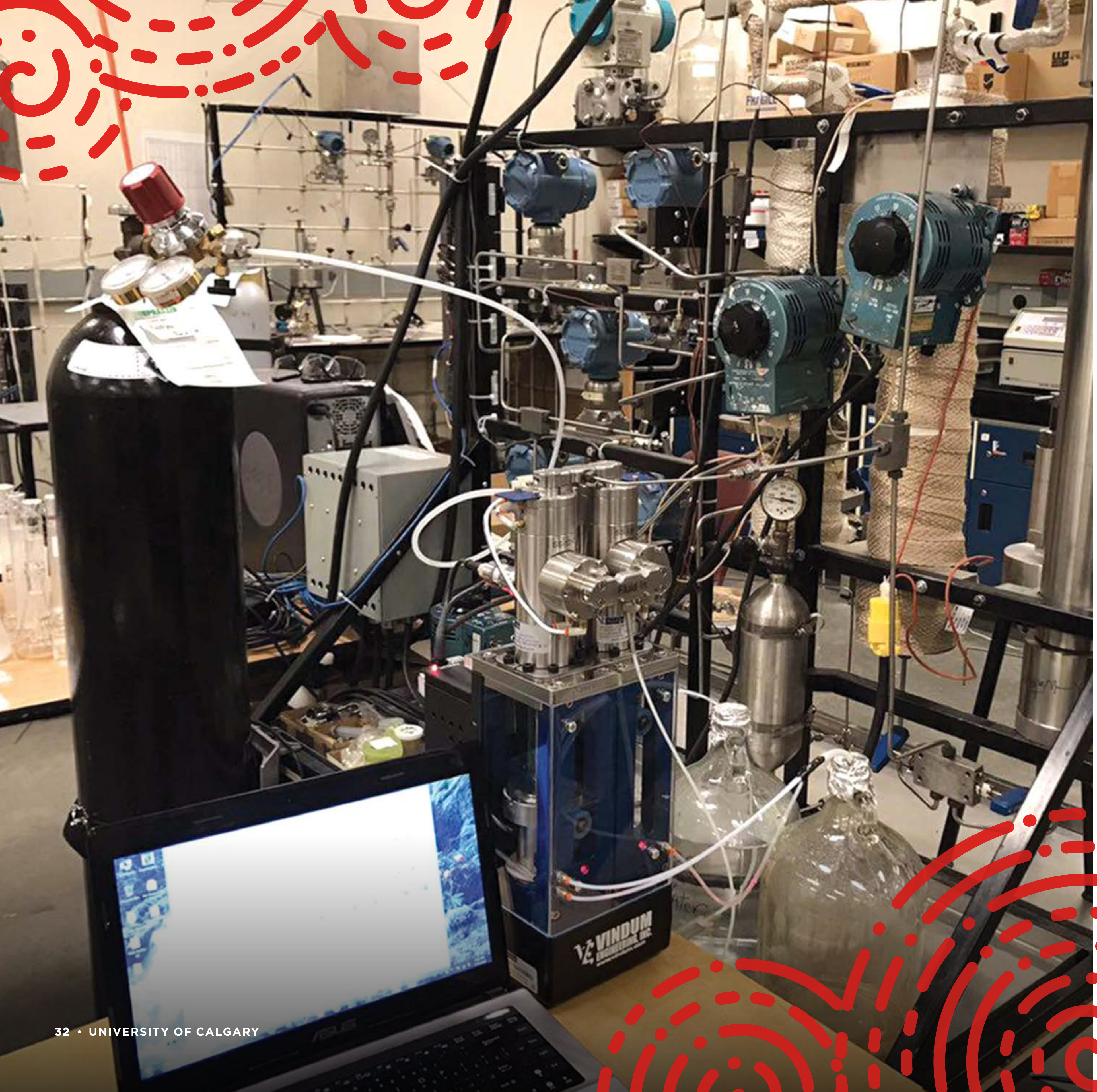
Solvent addition to steam is a promising pathway for making the steam-assisted gravity drainage (SAGD) process more energy efficient. Although the current focus of industry in solvent addition is on bitumen viscosity reduction via simple dilution, it may be possible to obtain even more dramatic improvement in energy efficiency by inducing *in situ* phase separation. If a process can be developed in which the injected solvent induces precipitation of immobile heavy hydrocarbons from the bitumen, the remaining liquid would be vastly more mobile and easier to produce to surface.

Research strategy

The goal of the project is to examine *in situ* phase separation of solvent and bitumen mixtures into light and heavy ends. The light ends should have much lower viscosity than that of the original bitumen which will enable production of oil to surface.

Desired outcomes

The desired outcome is identification of a tailored solvent composition that will induce precipitation of heavy hydrocarbons in immobile solid form, so that they will remain in the reservoir while the remaining oil that is now vastly more mobile will migrate to production wells. This will make the gravity drainage process more energy efficient and less damaging to the environment.



Thermal solvents for *in situ* phase separation

Sajjad Esmaeili
PhD student

Introduction

The steam-assisted gravity drainage (SAGD) processes are the most commonly applied technique to recover heavy oils and bitumen from the reservoirs in Canada. In using SAGD the high-temperature condition may considerably affect the flow characteristics due to altering the rock/fluid and fluid/fluid interactions such as the interfacial tension (IFT), contact angle and relative permeability. The importance of reliable relative permeability data under this condition, along with its scarcity in the literature, motivated the creation of this project. The attempt is to conduct two- and three-phase relative permeability measurements under SAGD conditions and a proposed new relative permeability model which are useful for reservoir simulations and economic evaluation of these processes.

Results

The research team reviewed studies that measured the relative permeability at elevated temperatures, though there are very few reported studies for bitumen systems. This review resulted in three manuscripts, two of which have been published in peer reviewed journals. Next, the team focused on the measurement of oil/water relative permeability over a wide range of temperature up to 215 C using a viscous oil (PAO100) to test the apparatus and figure out possible problems during such measurements before employing a real bitumen. These preliminary measurements were successfully completed and show significant effect of temperature on relative permeability. For the next stages, the team will expand their measurements to the bitumen (Athabasca)/water and bitumen/gas systems.

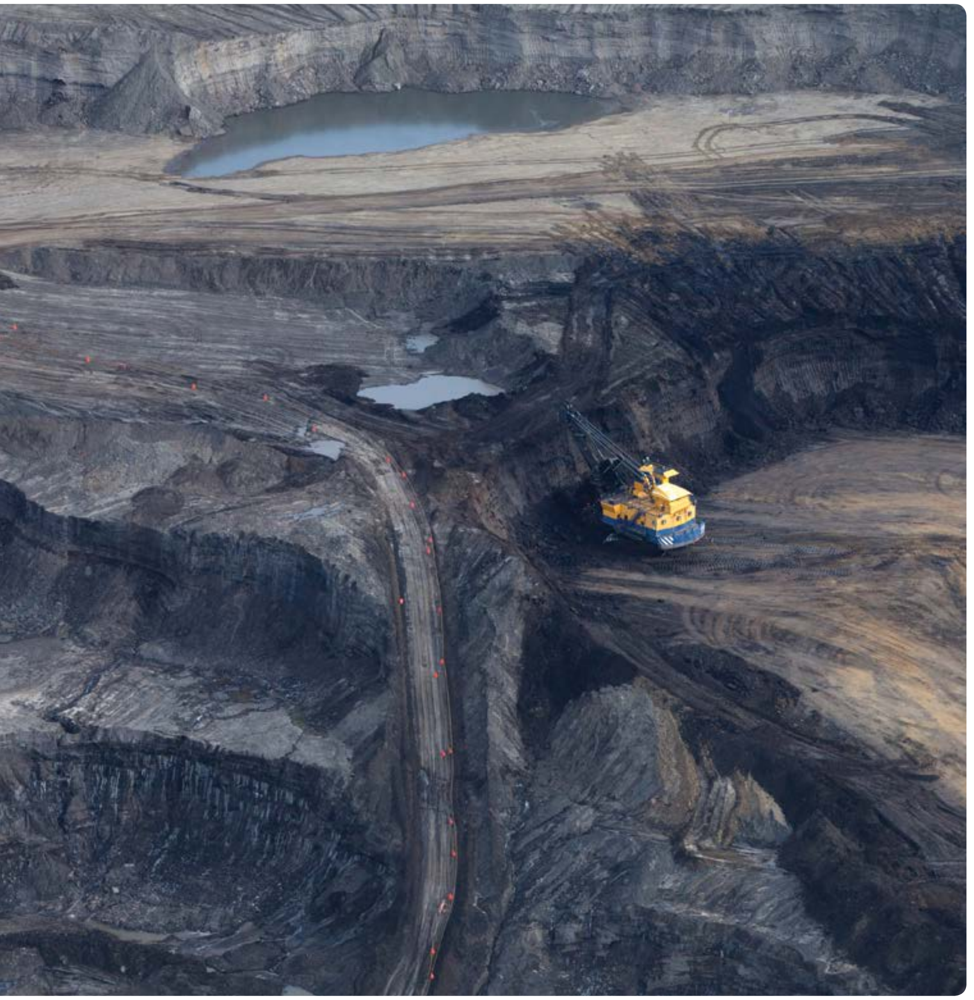
Conclusions

The primary results clearly demonstrate that in a viscous oil system, with increasing temperatures:

- The irreducible water saturation increases.
- The residual oil saturation significantly decreases.
- The water endpoint and the oil endpoint increase.
- The relative permeability to oil increases and the relative permeability to water tends to be reduced.

RESERVOIR CHARACTERIZATION FOR IMPROVED WELL PLACEMENT LEADING TO REDUCED EMISSIONS

Stephen M. Hubbard



Background

The oil sands deposits of the McMurray Formation are characterized by extreme lithologic heterogeneity, which is a primary control on bitumen recovery. A geo-realistic reservoir model is needed to take into account this multiscale heterogeneity, which will enable improved capability to place wells, and ultimately, improve steam conformance. Well placement and completion design are often not optimized relative to reservoir geology and thus do not perform to their maximum possible ability. Through this initiative, emission intensity during the recovery processes will be minimized.

Research strategy

Leverage a particularly well-constrained dataset of 3D seismic data, drill cores and wireline logs suites from the Surmount asset of northeastern Alberta to build the most geologically realistic reservoir model for the Athabasca Oil Sands to date.

Desired outcomes

Geological heterogeneity that impacts flow at multiple scales is difficult to constrain in *in situ* oil sands projects, and it is commonly simplified to facilitate reservoir simulations. The detailed model that stems from reservoir characterization efforts will enable alignment of well placement and completion design with reservoir geology, providing the foundation for next generation adaptive well simulations, and ultimately lead to improved design and lowered emission intensity in development projects across the province.

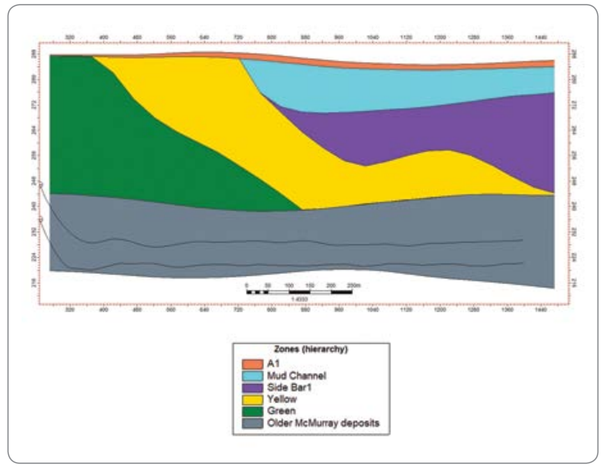
Reservoir characterization for improved well placement leading to reduced emissions

Siavash Nejadi
Postdoctoral Fellow

Introduction

The purpose of the study is to construct detailed static and dynamic reservoir models for meandering fluvial deposits in Athabasca Oil Sands. The geological model not only reflects the complex rock properties in three-dimensional space but also includes spatial distribution characteristics of inner structural elements. Individual meander-belt elements are mapped using seismic and well data (core, well logs, dip meter, formation micro-imager) and geostatistical simulations are constrained to the interpreted geobodies.

The integrated workflow extends reservoir characterization to reservoir simulation, production optimization and evaluation of the performance of *in situ* recovery techniques. The probabilistic nature of the study legitimizes quantifying the uncertainties and identifies associated risks for different development strategies.



Results

Identification and characterization of depositional elements in the McMurray Formation has important implications for reservoir prediction and development of oil sands resources. Widely spaced and sparse subsurface data combined with the poor quality of the seismic information in older McMurray deposits is a significant challenge to the study.

Results show that in contrast to the traditional workflows, constraining rock properties to deterministically interpreted structural elements reduces uncertainties in model parameters and enhances predictive capabilities of modelling. These include the ability for improved placement of the well pads, infill drilling well locations and optimization of downhole well completions tools. This leads to higher bitumen recovery at lower emissions (steam to oil ratio), and at the same time reduces capital costs by means of using an optimal number of wells with the finest completion equipment.

Conclusions

A detailed geological model undertaking a thorough evaluation of the key subsurface uncertainties is mandatory to design an overall development plan in meandering fluvial deposits in Athabasca Oil Sands.

Implications for reservoir development include improved well placement and production optimization constrained to geological features of the formation.

Developing advanced wellbore completions and optimizing downhole tool settings is critical to achieve optimal steam distribution in heterogeneous oil sand reservoirs for optimal recovery.

Dr. Siavash Nejadi, PhD, acknowledges Schlumberger for providing academic licenses for the Eclipse reservoir simulator and Petrel, and ConocoPhillips for the data for the field case study.

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

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 emerging technologies using life cycle assessment (LCA) and optimization

Zainab Dadashi Forshomi
PhD student

Introduction

This project uses a combination of life cycle assessment and optimization techniques to develop a tool for emerging technology assessment. The objective of the proposed framework is to assess the economic and environmental impacts of adopting emerging technologies, such as solvent assisted extraction and partial upgrading, in oil sands production compared to the existing technology pathways. Considering the uncertainties in the performance characteristics of emerging oil sands technologies, oil market and energy price, this framework intends to inform the investment decision making in oil sands production by determining the conditions under which emerging oil sands technologies become competitive alternatives in the global oil market.

Results

Preliminary results show that solvent assisted extraction has great potential for improving the economic and environmental impacts of the oil sands production (from extraction to refining and end use). *In situ* upgrading is another emerging technology that has significant impact on reducing the greenhouse gas (GHG) emissions of oil sands production. Additionally, partial upgrading technologies can become competitive alternatives for upgrading and dilution pathways under certain conditions.

The results of the analysis show that the basis of calculation for total profit and total GHG emissions of the oil sands production pathways can affect the choice of the optimal pathway significantly, i.e., if the calculations are done based on the flowrate of the refinery products, full upgrading pathway becomes the most profitable option compared to dilution and partial upgrading. If the calculations are done based on the bitumen flowrate, dilution pathways are more profitable than full upgrading.

Conclusions

Mathematical modelling and optimization of the entire oil sands supply chain allows for:

- A consistent comparison between different oil sands production pathways with respect to life cycle GHG emissions and cost.
- Creating a basis for decision making in oil sands industry by including uncertain market conditions and variable energy price forecasts.

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 our 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 assessment 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 Kelly MacDougall and Lydia DiCaprio are the Research Associates. Other University of Calgary faculty members involved in the projects under Theme 2 are Profs. Bernhard Mayer, Jeffrey Priest, Cathryn Ryan, Daniel Trad, Joule Bergerson, Shengnan (Nancy) Chen, Chris Hugenholtz, Ke Du, Kristopher Innanen, Per K. Pedersen, Steve Liang, Tatyana Plaksina and Hersh Gilbert.

CAN WE MITIGATE AND MANAGE RISKS OF INDUCED SEISMICITY?

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

Research Team 2: **David Eaton,** Shengnan (Nancy) Chen,
Jeffrey Priest, Mirko van der Baan (UAlberta), Japan Trivedi (UAlberta)
Shawn Maxwell (Industry), Patrick 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 millimeters to 10s of kilometers 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?

Microseismic monitoring of a Duvernay hydraulic-fracturing stimulation, Alberta Canada: Processing and interpretation guided by finite-difference synthetic seismograms

Germán Rodríguez-Pradilla
PhD student

Introduction

This project has four main research topics: (1) Finite-difference modelling of microseismic events in shale-gas reservoirs in western Canada. (2) Reservoir characterization of a shale reservoir from seismic and microseismic data to forecast the hydrocarbon production after a hydraulic-fracturing stimulation. (3) The application of the signal duration and radiated energy methods for magnitude estimation of microseismic events. (4) Ground motion and seismic-hazard analysis of induced seismicity sequences associated with multi-stage hydraulic-fracturing stimulations in Western Canada.

Results

Germán Rodríguez-Pradilla has been developing a processing workflow to model the occurrence of microseismic events and to detect real seismic events from passive seismic datasets acquired during several hydraulic-fracturing stages in a shale-gas reservoir in Western Canada. Some of the obtained results have been published in international journals and conferences, and some others are in preparation to be submitted for publication. All these topics and results are fundamental components of his doctoral research.

Conclusions

Processing large-volume passive seismic datasets, as those acquired to monitor hydraulic-fracturing stimulations in unconventional reservoirs, is typically time-consuming and computationally expensive.

To overcome this, the research group at the University of Calgary (Microseismic Industry Consortium) has always provided all the necessary tools (hardware and software) and the support from high-level researchers who are also part of the research group.

Industry partners have also been receptive when reviewing the obtained results from this work.

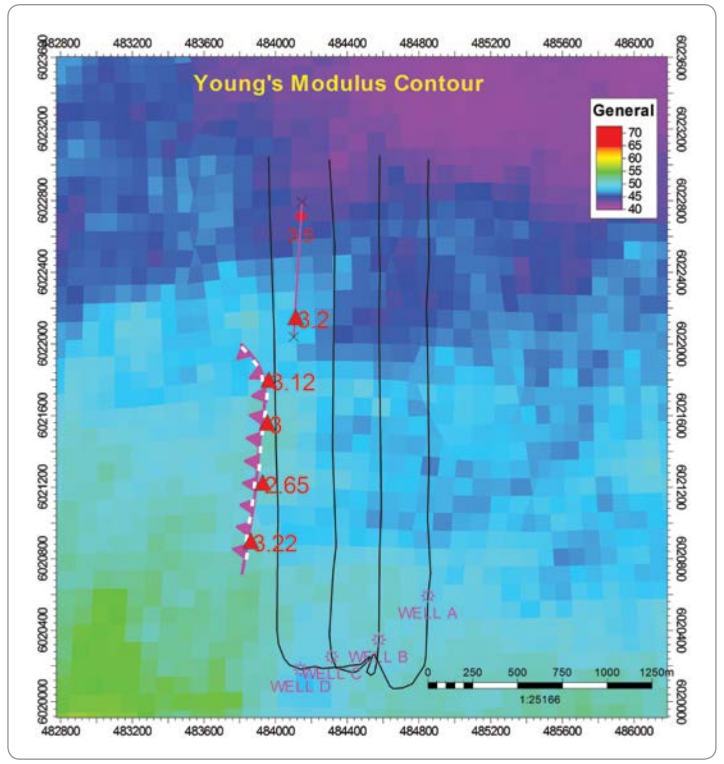
Germán Rodríguez-Pradilla acknowledges TransAlta Corp. and Nanometrics Inc. for providing access to the seismicity detected with the regional seismological network installed in Alberta. The research team also thanks the operator companies of the studied shale-gas reservoir, for supporting the near-surface local seismic monitoring program acquired under license using MicroSeismic Inc.'s BuriedArray® design.

Can we mitigate and manage risks of induced seismicity?

Hui Gang
PhD student

Introduction

A thorough literature review on the induced seismicity has been conducted and it was found that hydraulic fracturing is responsible for triggering seismicity activity, or even some earthquake events, in the Western Canada Sedimentary Basin. The current research concentrates on the case study of four horizontal wells to investigate the relationship between hydraulic fractures and induced seismicity. This comprehensive and challenging approach integrates geology, geophysics, geomechanics and reservoir engineering to interpret the mechanism of fault activation and induced seismicity. Also, the seismic hazard analysis for induced seismicity can help regulate the treatment scale of hydraulic fracturing, such as pumping volumes and treatment pressure.



Results

In the case study, stratigraphic features were studied based on formation tops of 42 surrounding wells. Three different geomechanical sublayers were classified within the Duvernay formation. Reservoir properties were characterized using core analysis and well logs. The same method was also applied to reservoir geomechanics, whose distribution matches well with that of 3D seismicity property inversion. The hydraulic fracturing process integrating the above models was simulated to characterize hydraulic fractures parameters. The half-length for stage one of Well D (220 meters) is similar to that of monitoring fractures (250 meters). By comparing the time-space sequence of induced seismicity events with hydraulic fracturing treatment, the results suggest that two events of induced earthquake with moment magnitude (Mw) 3.5 [total vertical depth (TVD) 3300 meters] and Mw3.2 (TVD4900m meters) respectively, could be triggered by hydraulic fracturing of stage five, which also means that the fault developing from the top 3210 meters to the bottom 4929 meters is activated.

Conclusions

The most significant parameter controlling induced seismicity in the Duvernay play near Fox Creek is the large fracturing fluid volume and high treatment pressure.

The direct fluid pressure effects of injection lead to an increase in pore pressure along the fault, which causes reactivation of the existing fault.

Hui Gang acknowledges Nanometrics for providing the reported seismicity detected with the regional seismological network near Fox Creek. The research team is also grateful to GeoLOGIC for providing the completions and fracturing data and well logs.

Can we mitigate and manage risks of induced seismicity?

On ground motion effects of induced seismicity on buried pipelines: Probabilistic approach

Sahar Ghannadi
Postdoctoral Fellow

Introduction

This project studies factors that affect the likelihood of damage to pipelines due to ground motion. Ground motion due to induced seismicity is not currently evaluated in most hazard assessments of pipelines. Failures categorized as *external interference* follow the normality line at inversed safety factor (1/SF) greater than 0.3, which means that when induced seismicity creates strain of 30 per cent of the pipeline allowable strength (presented on the basis of strain-based design), failure will be initiated that may only present up to 60 days after the original event. One of the most critical lessons learned is the need for including seismic planning for pipeline design and maintenance.

Results

In this project, comparison of the relative contributions of the *external interference, corrosion cracking,* and *defect and deterioration* is presented. The failures associated with *external interference* in the z-value versus probability graph are following the linear normality line that shows the external forces are dominantly caused by induced seismicity. Such normality cannot be seen in failures categorized in *corrosion cracking* and *defect and deterioration*. Failure due to corrosion should not be affected by induced seismicity. This result indicates that induced seismicity events could pose failures due to ground motion and longitudinal strains along the pipelines. The normality test shows that the SF of 10 (or 1/SF of 0.1) can cause failures, and to mitigate failures SFs greater than 10 should be used.

The results of this analysis indicate that further improvement in seismic integrity should be considered for pipelines that are not designed for dynamic forces or even simply increase SF by 10 or lower, and the allowable strain by 0.0003.

Conclusions

In this work, a probabilistic approach is used to understand and validate if induced seismicity can cause failure along the pipeline.

With the growth of shale gas development in eastern British Columbia and the potential for localized strong ground motions from these shallow induced seismicity events, it can pose an increased hazard to major pipelines.

In case a specific mechanism is causing the failure, both load and capacity (or strength) are normally distributed. Similar trends can be seen in safety factor.

Alternatively, if the mechanism of such failure is unknown, but the safety factor is calculated on the basis of load and capacity formulation, for that mechanism is normally distributed, then the mechanism is dominantly controlling the failure.

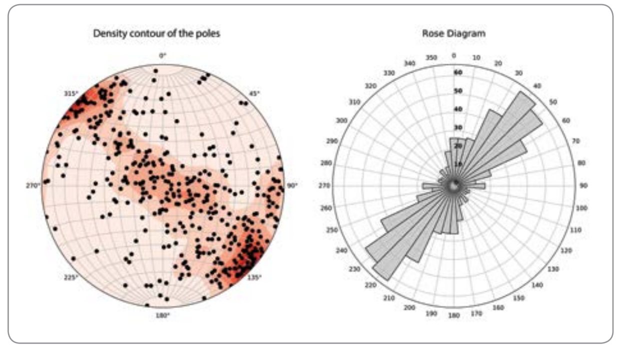
Can we mitigate and manage risks of induced seismicity?

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

Scott Harold McKean
PhD student

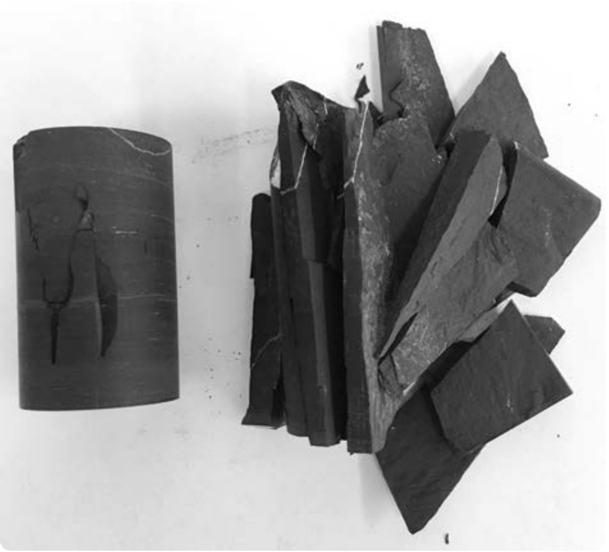
Introduction

Scott McKean's research focuses on the characterization of the subsurface using disparate types of evidence including microseismic data, frac hits and outcrop analogues. The main goal of his research is to constrain the parameters in the subsurface to predict how hydraulic fractures connect to faults and ultimately, what the probability of slip on a pre-identified fault is. This is a difficult problem because of the heterogeneity of the subsurface and the high computational demands required for stochastic numerical modelling, as well as the indirect nature of the evidence used to constrain these complex models.



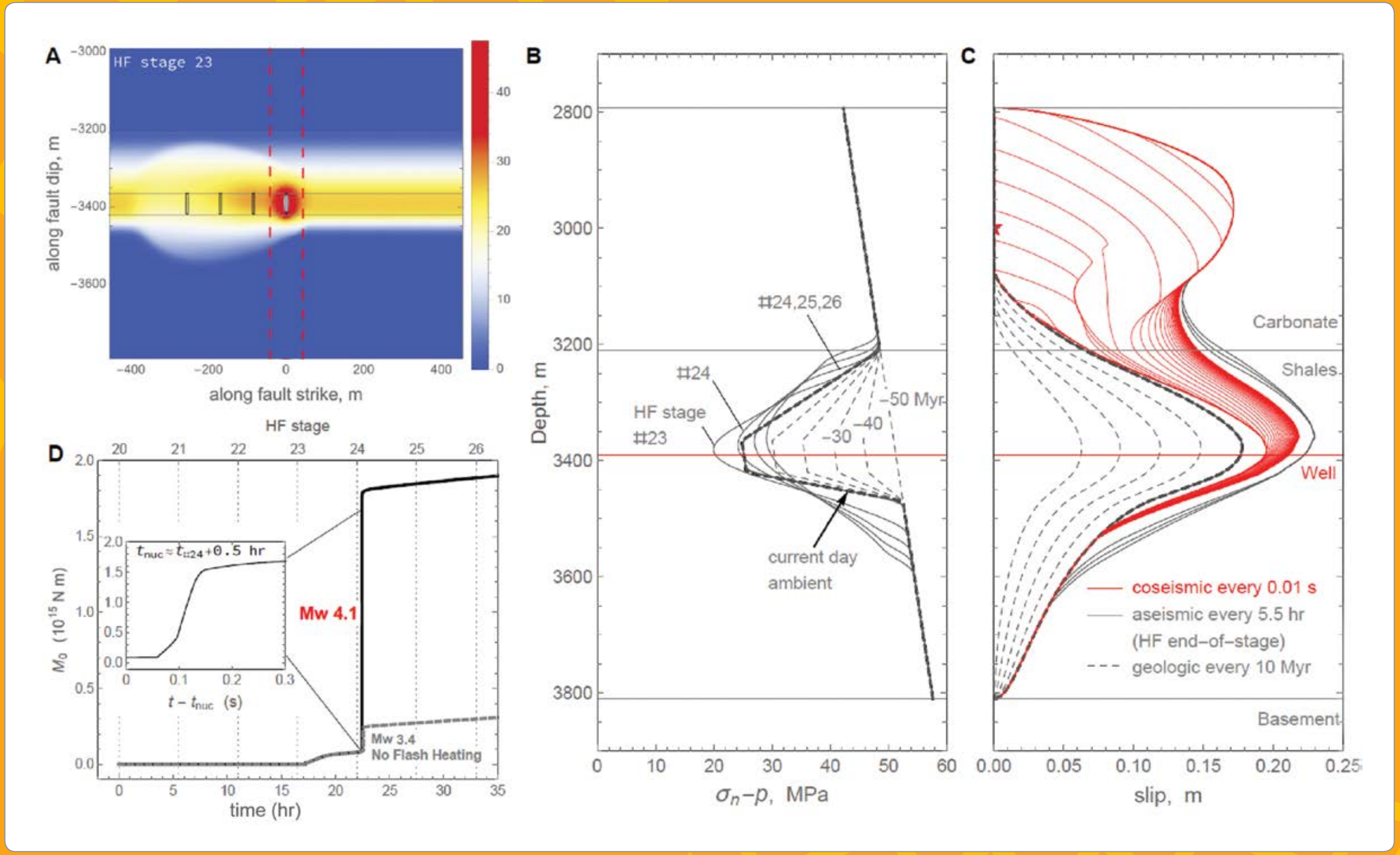
Results

Scott has shown that it is possible to use unsupervised machine learning (clustering) to constrain discrete fracture networks in a physically plausible way using microseismic data. He has also reviewed the background on interwell connectivity (i.e. frac hits) and has shown how they may be able to constrain the diffusivity of subsurface fractures. Scott has successfully ran advanced triaxial tests on outcrop analogues of the Duvernay and the basement that underlies it and challenged some of the preconceived notions on post-peak failure. He attempted a Bayesian logistic regression study in order to constrain fault strength parameters (cohesion and friction), but the approach was unsuccessful as the binary pass/fail data from the earthquakes did not have enough information to properly conduct the Bayesian analysis.



Conclusions

Gaussian mixture model based clustering can successfully identify physically plausible discrete fracture networks from dense microseismic data.



Can we mitigate and manage risks of induced seismicity?

Thomas Eyre
Postdoctoral Fellow

Introduction

In this new model for hydraulic-fracturing induced seismicity, fluid injection accelerates a seismic slip on nearby faults in the reservoir and surrounding formations which, according to geomechanical analysis, are expected to exhibit stable sliding. This work has major impact in the field as it constitutes a fundamental shift from the current paradigm. Along with the model, Thomas Eyre's research is leading the development of a new computational toolbox to aid in producing quantitative mitigation and response plans by combining reservoir-simulation methods with advanced geomechanical and seismological computational tools. The aim is to commercialize this with help from Innovate Calgary, the technology transfer centre at the University of Calgary.

Results

The research team carried out detailed analysis of a novel high quality microseismic dataset showing fault activation during a hydraulic fracturing treatment. Unfortunately, the subsequent manuscript was rejected from the Bulletin of the Seismological Society of America after second round reviews. The manuscript is now being redrafted and prepared for submission elsewhere. The new model has been submitted (and rejected) to several high-impact journals. The research team believes in its importance and the model is currently submitted to Science Advances. Thomas is working on another related project on the long-lived nature of some induced seismic swarms which will likely result in at least one publication. The software development project is now moving forward thanks to a collaboration with SAIT. Thomas's work has also resulted in eight conference presentations/publications.

Conclusions

Developed an alternate model for hydraulic-fracturing induced seismicity which is a major shift in the current paradigm.

The computational toolbox project is moving forward at an accelerated pace, with the aim of a full prototype by summer 2019.

Dr. Thomas Eyre, PhD, acknowledges Repsol Oil & Gas Canada Inc. for providing microseismic data, which were processed by Magnitude; XTO Energy Inc. for providing data which were processed by ESG Solutions; TGS Canada Corp. for providing 3D multicomponent data used in this study; TOC data were measured by Weatherford and XRD data were collected by Chevron; these data were sourced from the Alberta Energy Regulator database; and the software development team at SAIT and Innovate Calgary for their assistance in this project.

SUSTAINABLE HYDROCARBON RECOVERY FROM LOW PERMEABILITY RESERVOIRS

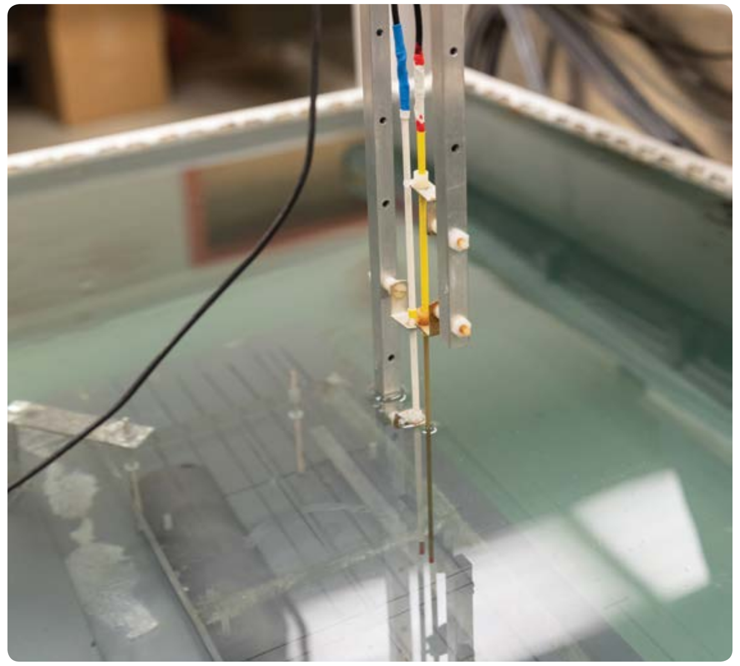
Kristopher Innanen, Shengnan (Nancy) Chen, Tatyana Plaksina, Daniel Trad, Ian Gates

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

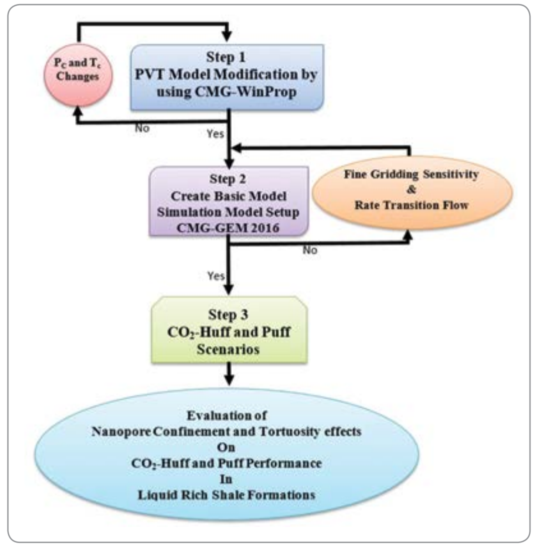
Combinations of methodologies for seismic acquisition will be validated in laboratory studies and in field scale trials. Other related projects will be generating methodologies for pre-processing data and for producing properly parameterized full-waveform inversion (FWI) algorithms; here, field and lab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

Sustainable hydrocarbon recovery from low permeability reservoirs

Abdolmohsen Shabib-Asl
Postdoctoral Fellow

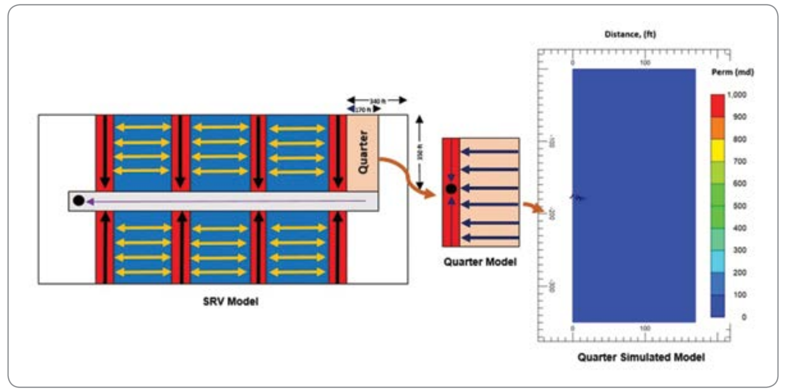
Introduction

This work investigates a spectrum of problems associated with modelling enhanced oil recovery (EOR) processes using CO_2 injection in shale/tight oil reservoirs. The research team has developed better approaches to unconventional oil evaluation as a foundation to which CO_2 EOR is then applied. Currently the research focuses on improved unconventional reserve evaluation using the systematic decline curve analysis (DCA) model that affects ultimate oil recovery. One of the effects that the team considers while modelling CO_2 EOR is the effect of pore confinement on fluid properties, which is usually ignored in shale simulation experiments. This study demonstrates how modelling pore confinement changes the pressure volume temperature (PVT) model and ultimately leads to higher oil recovery in ultra-tight formations.



Results

To investigate the nanopore confinement effect during the CO_2 huff-n-puff study, the team used compositional reservoir simulation to model the effect of pore confinement and assess the performance of CO_2 huff-n-puff in hydraulically fractured shale formations. First, they built and tested a quarter model with fine gridding to capture transient flow during production simulation. Second, they examined the accuracy of the model using rate transient analysis (RTA). Third, they conducted a sensitivity study on several key parameters such as CO_2 injection rate, injection time, soaking time and injection cycles. Finally, they assessed the results and concluded that the performance of CO_2 huff-n-puff depended on these parameters and that neglecting pore confinement had a serious impact on production forecasts from unconventional assets.



Conclusions

Simulation results are dependent on the grid block size and the number of refinements.

Fine gridding improves the accuracy of the simulation results.

Pore confinement has a significant effect on oil recovery when the pore size is considerably less than 10 nanometers.

Sustainable hydrocarbon recovery from low permeability reservoirs

Energy and emissions of unconventional resources

Evar Chinedu Umeozor

PhD student

Introduction

As yet, the development of unconventional resources remains unclear in the context of economic, energy efficiency, and environmental impacts. The intent of this project is to develop new assessment methods to quantify environmental, energetic and economic impacts of unconventional resources development. The research team has developed new modelling and assessment methods to quantify impacts of shale gas, oil sands and CO_2 utilization developments. By quantifying impacts of resource development, they aim to identify preferred alternatives for new system designs and improvement opportunities in current design and operational practices (in terms of energy efficiency, environmental, and economic impacts). The results impact both business decisions and policy processes.

Results

There are four main outcomes from Evar Chinedu Umeozor's research. (1) The development of a new model to quantify environmental and economic impacts of shale gas development considering various scenarios for conservation of potential emissions during well completions. (2) The development of methods to determine contributions of preproduction operations to energy use and emissions during shale gas development, highlighting the major elements in the operations to be optimized in order to improve overall performance. (3) The comparison of energy, emissions and economic impacts of emerging oil sands production processes and technologies, identifying opportunities for operational improvements through solvent based recovery. (4) The identification of mitigation options for the environmental impact of growing unconventional resources development as it pertains to climate change mitigation, showing the role of CO_2 utilization as mitigation strategy to convert emissions to products.

Conclusions

There is potential for profitable implementation of emission capture during shale gas development.

New models highlight contributions of preproduction operations to overall energy use and emissions during shale gas development. There is a need to focus on drilling and completions energy and emissions impacts as well as those from flowback.

An assessment of emerging oil sands processes show that solvent process design is promising but requires cheap solvents and additional recovery mechanisms beyond that of gravity alone.

CO_2 utilization is a potential climate change mitigation strategy for converting emissions to products like polymers and chemicals.

Evar Umeozor acknowledges Drilling Info for supplying its database on hydraulic fracturing operations for North America.

Sustainable hydrocarbon recovery from low permeability reservoirs

Marcelo Guarido de Andrade

Postdoctoral Fellow

Introduction

Dr. Marcelo Guarido de Andrade, PhD, is currently participating in two different project branches: (1) Physical modelling laboratory focused on simulations for seismic-while-drilling (SWD) and full waveform inversion (FWI) studies. For this, the laboratory needed to be upgraded so the simulations are closer to the real world, but with all the parameters under control. (2) Machine learning focused on the extraction of rock properties and/or classification from well logs, and the identification of targets using seismic data. The goal is to create workflows that will give new insights to the interpreters. Marcelo also created a new FWI scheme that is cheaper than the current method.

Results

New digitizers and transducers were purchased for the SWD and FWI simulations in the laboratory. Models are being built for the SWD simulation. Figure 1 is the model proposed for the simulation and Figure 2 is the schematic drawing for its construction. Machine learning methods were used on well logs for facies classification with 60 per cent accuracy (very high), and Figure 2 shows its results on the validation well. Deep learning algorithms were applied for salt identification on seismic images. A cheap, but high resolution output velocity model, FWI scheme was developed and tested on land seismic data. Figure 3 shows the initial and inverted models.

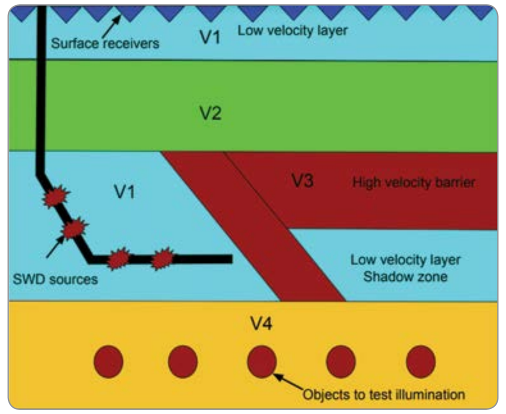


Figure 1

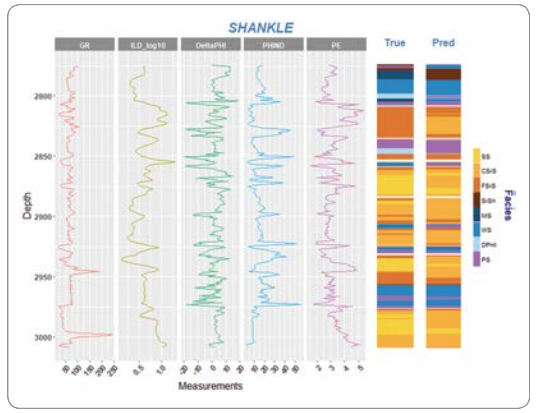


Figure 2

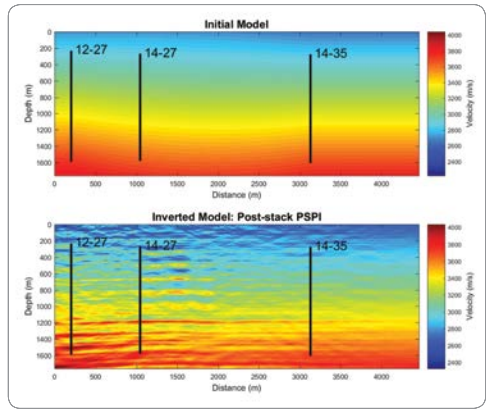


Figure 3

Conclusions

The physical modelling laboratory was successfully updated and is currently running the SWD simulations.

Machine learning for facies classification using well logs gives trustful results, helping interpreters with their work.

Using deep learning for salt identification on seismic images has high accuracy and can help provide fast and easy insights for interpreters.

The new FWI scheme (FastWI) is cheap and requires low computational resources but works mainly for P-wave velocity inversion.

Sustainable hydrocarbon recovery from low permeability reservoirs

Shuhua Wang
Postdoctoral Fellow

Introduction

CO_2 flooding is one of the most preferred enhanced oil recovery (EOR) methods for producing oil from various kinds of reservoirs because of its favorable EOR mechanisms. In this project, the research team is focusing on the performance optimization of CO_2 EOR and storage in unconventional tight reservoirs. The biggest challenge is to develop a multi-objective optimization algorithm which is capable of not only maximizing the hydrocarbon productions, but also increasing the CO_2 storage capability in unconventional tight reservoirs. Such a multi-objective optimization process can provide a useful tool for engineers to co-optimize the operations of CO_2 EOR and storage in unconventional oil reservoirs.

Results

A comprehensive optimization process has been developed to optimize the production performance of the entire production lifespan for the CO_2-water alternating gas (WAG) EOR process. The newly developed comprehensive optimization process not only optimizes the WAG parameters including the WAG half-cycle length, gas and water injection rates, and bottom hole pressures (BHPs) of producers, but also the start-up times of water flooding and the following CO_2 WAG process.

For the perspective of EOR, CO_2 huff-n-puff performs better than CO_2 flooding for low permeability reservoirs, whereas it is not that effective in terms of CO_2 storage with comparison to CO_2 flooding. It might be more effective for both EOR and storage by applying CO_2 huff-n-puff EOR during the early stage of development of an unconventional multi-well pad, then switching to CO_2 flooding in the later stage.

Conclusions

Results demonstrate that the oil recovery and net present value (NPV) of the optimized CO_2 WAG process are increased by 23.4 per cent and 51.3 per cent, respectively, in comparison to the optimal case obtained by the conventional WAG optimization process.

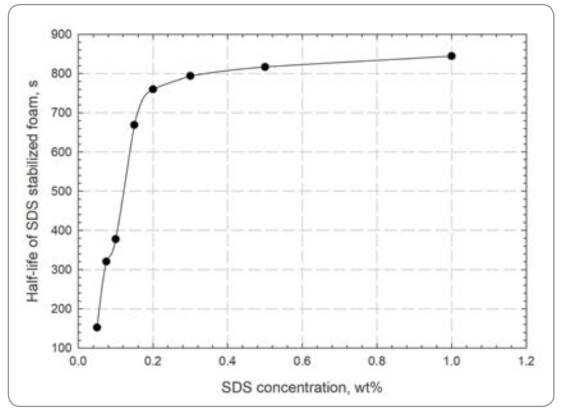
The macroscopic sweep efficiency of the optimal CO_2 WAG process can be sufficiently improved by properly adjusting the injection-production parameters, which is justified by the decrease of the remaining oil saturation distribution.

Sustainable hydrocarbon recovery from low permeability reservoirs

Sixu Zheng
Postdoctoral Fellow

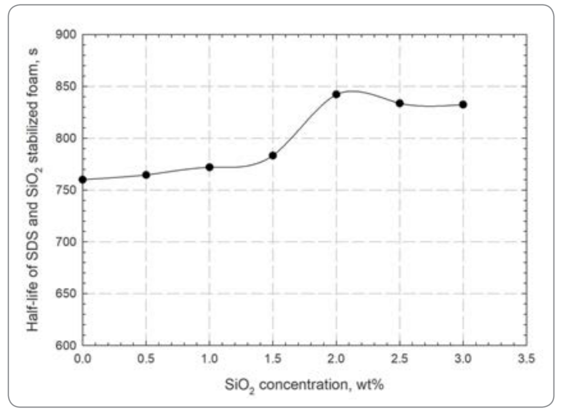
Introduction

The conventional water-based hydraulic fracturing fluids consume a large amount of water and may cause severe formation damage during fracturing processes in tight oil and gas reservoirs. Foam-based fluids are promising hydraulic fracturing fluids that can reduce water consumption and mitigate formation damage. In this project, the research team is examining different foam-based hydraulic fracturing fluid systems and quantifying their stability, sand-carrying capacity and compatibility with formation rocks and fluids. A proper fracturing fluid system will be selected and optimal concentrations of the additives will be determined. The scientific findings will promote a more economical and eco-friendly manner of hydraulic fracturing.



Results

Statistical analysis for the stimulation and production data of over 5,000 wells in the Montney formation shows that multi-phase fracturing fluids had better performance on fluid leak-off than that of a single phase fracturing fluid (i.e., water). The surfactant sodium dodecyl sulfate (SDS) and three types of nanoparticles [silicon dioxide (SiO_2), aluminium oxide (Al_2O_3) and ferric oxide (Fe_2O_3)] have been examined to stabilize the foam. It is found that the optimal concentration of SDS is 0.2 weight per cent to stabilize foam. The stability of SDS-stabilized foam was first increased with salinity until 2.0 weight per cent of sodium chloride (NaCl), and then it sharply decreased. Among these nanoparticles, the addition of nanoparticles into SDS solution can improve foam stability, while Al_2O_3 and Fe_2O_3 decreased the half-life of foam systems. The SDS and SiO_2 stabilized foam that can bear high NaCl concentration. The stability is increased when the NaCl concentration is increased from 0.5 weight per cent to 3.0 weight per cent.



Conclusions

Foam-based fracturing fluids have superior performance on fluid leak-off over that of a single phase fracturing fluid.

Among the three examined nanoparticles (i.e., SiO_2, Al_2O_3, and Fe_2O_3), the addition of SiO_2 into SDS is able to improve foam stability.

SDS-SiO_2 stabilized foam can withstand a higher salinity.

Sustainable hydrocarbon recovery from low permeability reservoirs

Hydraulic fracturing physical modelling

Zheng Li
PhD student

THEME 2: TIGHT OIL AND GAS

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. The research team uses ballistic gel as the medium for hydraulic fracturing and exerts different stress fields on the gel to examine how hydraulic fractures grow within the media. The team had many challenges placing intact wells within the gel but now have procedures to do this reliably. The results from the experiments will be scaled-up to be applied in a real field-scale reservoir.

Results

The main outcome from the research so far has been successfully fracturing in both vertical and horizontal directions. The team has examined the effect of gel stiffness on hydraulic fracturing and they have compared the results from the experiments to theory, demonstrating a match between the two.

Conclusions

- Using ballistic gelatin as a new transparent material to physically simulate hydraulic fracturing is feasible.
- Fracture direction depends on minimum principal stress direction.
- The fracture propagating process in the physical gel model is well matched with the theory.
- The results in lab can be scaled up and used in real field applications.

Zheng Li acknowledges SAIT for their support on design of the hydraulic fracturing apparatus.

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

Bernhard Mayer, Cathryn Ryan, Chris Hugenholtz, Joule Bergerson, David Eaton, Roger Beckie (UBC), Aaron Cahill (UBC)

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?

How well quantified are fugitive methane emissions around Alberta's petroleum wells?

Jason Abboud
MSc student

Introduction

Quantifying fugitive methane emissions around leaky oil and gas wells is necessary to address climate change initiatives set out by the governments of Canada and Alberta. Fugitive methane migration that originates in the subsurface and migrates through the soil (gas migration) can manifest at surface either as (1) flow through surface casing and a vent assembly (surface casing vent flow) or (2) through cracks or fissures in well casing. This project used energy industry databases to evaluate how many petroleum wells in Alberta have been tested for fugitive methane migration.

Results

Test results from a relatively sparse subset of wells are available in a provincial database, but the rates are not well quantified and the database is poorly curated. As of 2017, an estimated 3.5 per cent of Alberta's wells have required gas migration testing and 58.2 per cent of wells have required surface casing vent flow testing prior to abandonment. Additionally, 14.5 per cent of wells have been abandoned without any fugitive methane migration testing. The research team concludes that fugitive methane emissions from petroleum wells testing are not well quantified in Alberta. Since wells with surface casing vent flow or gas migration cannot be legally abandoned, this issue is contributing to the increasing number of inactive and orphaned wells in the province.

Conclusions

Fugitive methane emissions from petroleum wells needs to be quantified, particularly for gas migration, since a small fraction of wells have required testing and the related database is not well curated.

Failure to understand and target fugitive methane migration has contributed to the liability of increased numbers of inactive and orphaned wells.

Jason Abboud acknowledges the Alberta Energy Regulators for generously sharing data at no cost.

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

Marshall Staples
PhD student

Introduction

The goal of the project is to design and implement an optimal unmanned aerial vehicle (UAV) path planning algorithm for a sniffer drone to determine the source location and flux of fugitive methane gas emissions in an area where possible leak locations are known. Challenges include designing a path planning algorithm that can use poor sensor data. With a limited payload capacity, drones are restricted to lighter sensors which are often still in development. There is usually greater uncertainty in the validity of the sensor readings of the lighter sensors.

Results

Marshall Staples is in the early phase of research, having started his PhD in May 2018. The next steps in this project include testing potential autonomous algorithms in simulation for the sniffer drone and testing/verifying the accuracy of sensors to be used on the sniffer drone. The sensors to be tested include wind sensors and methane gas concentration sensors. If it is found that there is an accuracy limit on the sensors, then the autonomous algorithm may need to be modified to become robust to sensor error.

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

Small footprint recovery from low permeability hydrocarbon resources

Mehdi Rezvandehy
Postdoctoral Fellow

Introduction

Expansion in exploitation of natural gas from shale gas reserves has raised public concern regarding the increase in greenhouse gas (GHG) emissions. Fugitive CH_4 emissions during drilling and well completion have been taken into consideration recently as a main source of emission. This work focuses on modelling the fugitive emissions in different locations to better understand the extent of these emissions across Western Canada. The spatial coverage of the surface monitoring network that provides *in situ* measurement are limited to a small fraction of the possible locations since the operation is costly and time consuming. The research team is waiting for *in situ* data; however, observations from satellites offer new data sources. Geostatistical technique is applied on satellite data in this work.

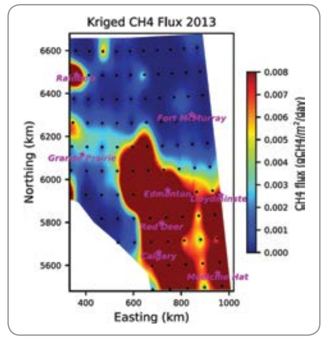


Figure 1

Results

The satellite observations are sparsely positioned have low resolution because of certain limitations including the observational mode of the satellite, and have noise and artifact in comparison with *in situ* measurement. Conventional geostatistical estimation is unable to model extreme low and high values and leads to smooth models without uncertainty quantification. In this work, geostatistical simulation, taking into consideration the uncertainty in input statistics, such as uncertainty in the histogram and variogram of data, is applied to high resolution models (Figure 1). This leads to a total CH_4 estimation with associated uncertainty and identification of locations with high probability of CH_4 emission and leakage (Figure 2). In the meantime, high resolution CO_2 from satellite data is being constructed that could lead to a better understanding of the agricultural cycle and the transport mechanisms. Reasonable monitoring methods to detect CO_2 concentrations can provide improved modelling and decision-making to enhance agricultural productivity.

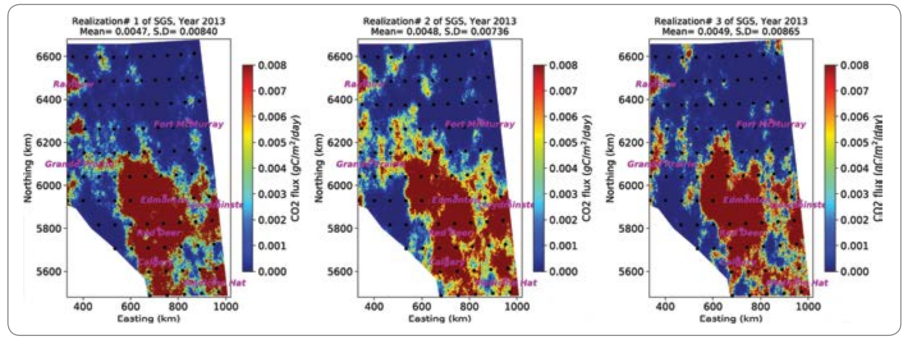


Figure 2

Conclusions

- Modelling high resolution GHG emissions in Alberta using sparse atmospheric data with consideration of uncertainty in input statistics.
- Using these methods it is possible to estimate the total CO_2 and CH_4 in Alberta.
- These methods can also be used to detect the areas with the highest probability of CO_2 and CH_4 emissions.
- Limit and customize ground-based measurements for future operation of fugitive gas detection.

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

Neil Fleming
MSc student

Introduction

Under the supervision of Prof. Cathryn Ryan, Neil Fleming is conducting research to better understand the subsurface movement and attenuation of natural gas from leaking energy wells. This project involves study of current methods used by industry for the detection of leaking wells and the spatial and temporal variability of the leaking gas. Information from this project can be used to aid in building an understanding of the mechanisms by which fugitive gas moves within the subsurface, including the potential impacts that leaking gas may have on fresh groundwater resources. In addition, information on gas movement and detection methods may influence and improve current industry practices.

Results

This project is currently in its first phase, which involves procuring legal access to energy wells for study. Team members have been working with various industry partners, including well owners, consultants, and service company representatives, for assistance in this process. Historic gas migration reports have been acquired for review and comparison.

Some field work was conducted between May and August 2018, where gas concentrations were measured around 6 leaking industry wells by 1-3 different specialists. Comparison of these methods, in addition to previously available gas migration reports, allow for analysis on the effects that different gas migration survey methods may have on detecting leaking wells. More intensive additional measurements were conducted around one of these wells to provide a better spatial understanding of the gas concentrations.

Conclusions

- Gas migration from leaky energy wells has a potentially significant but poorly understood impact to water quality and greenhouse gas emissions.
- There are variations in gas migration detection techniques used in industry.
- There are spatial variations in gas concentrations around leaking energy wells, both laterally and with depth in the soil.
- These differences in technique and occurrence may influence the detection of gas migration.

Neil Fleming acknowledges funding from the Petroleum Technology Alliance of Canada's Alberta Upstream Petroleum Research Fund, through a National Science and Engineering Research Collaborative Research and Development Grant. Other important external acknowledgments are for: The City of Medicine Hat, Turner Valley Gas Plant Historic Site, CG Engineering Ltd. and Aurora Land Consulting Ltd.

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

Gas migration field research project

Tiago Antônio Morais
PhD student

Introduction

The primary goal of this research is to evaluate the nature and extent of free and dissolved phase fugitive methane transport in the freshwater zone, the fundamental processes and mechanisms that govern its transport and attenuation, and the water quality and geochemistry implications of methane invasion into freshwater aquifers. The field research program (starting in the summer 2019) will design and install long-term monitoring of groundwater instrumentation to directly observe gas migration in both dissolved and free gas phases, and the effect of methane invasion on groundwater quality in the shallow zone. Currently, the biggest challenge is gaining access to energy wells with a lot of gas migration to perform a more detailed study.

Results

In summer 2018, Tiago performed several gas migration surveys around leaky oil and gas wells with Neil Fleming (an MSc student at the University of Calgary) to find a potential well for the second phase of this study (which will include a much more detailed monitoring program). Based on the high temporal and spatial variability of gas migration observed, the team will continue conducting these surveys to make sure they select the best well for the second phase.

Once the research team has selected the best well for further investigation, groundwater monitoring wells (multilevel sampling systems) will be installed around the selected well. The monitoring program will include physical, geochemical and isotopic characterization and their changes both spatially and temporally over the monitoring period (1-2 years). Tiago has already tested several commercial and customized total dissolved gas probes and diffusion gas samples in a groundwater monitoring well in Rosebud, Alberta during summer 2018, to verify if it would be feasible to use them during the second phase of this project.

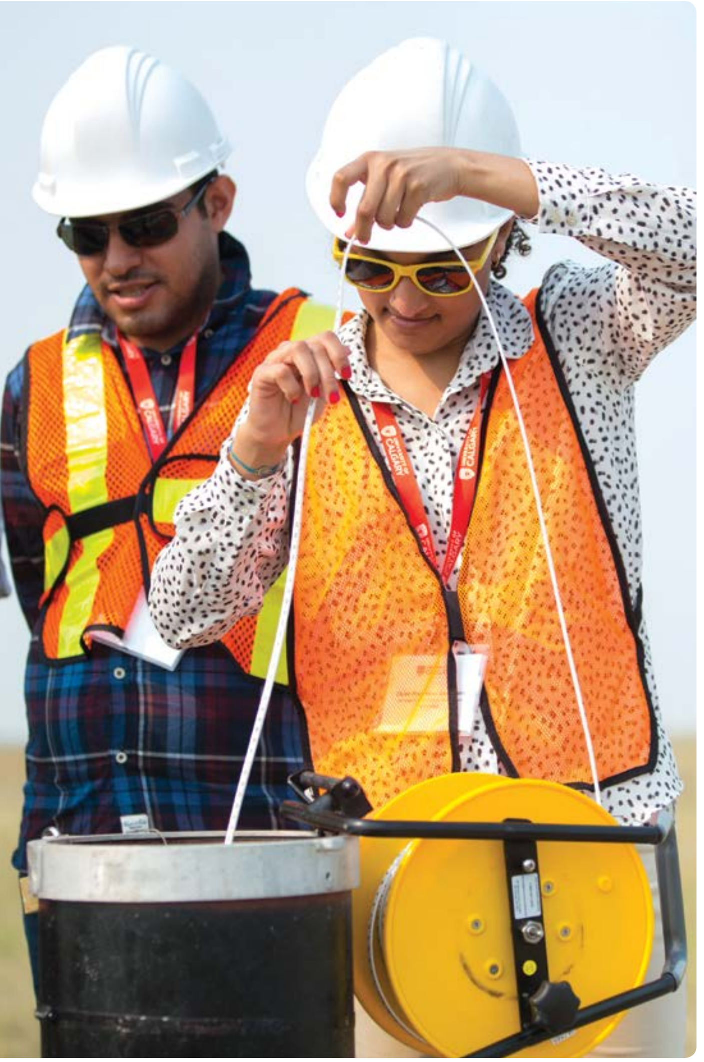
Conclusions

- Anecdotally it is understood that gas migration events around abandoned oil and gas wells are episodic.
- Leakage depths and anisotropy of the geologic medium appear to play a critical role in transporting methane.
- Long-term monitoring surveys are essential to estimate accurate total methane releases (groundwater+ atmosphere).

Tiago Antônio Morais acknowledges the City of Medicine Hat, AEP, and Pro Oceanus staff for their assistance.

FUGITIVE METHANE EMISSIONS

Bernhard Mayer



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. Concerns have been raised about the extent of greenhouse gas (GHG) emissions, especially CH_4, into the atmosphere associated with the production of shale gas from unconventional hydrocarbon resources (UHR) either by surface casing vent flows or via gas migration through the water-unsaturated soil zone outside of well casings, among others. Currently, there is a lack of effective and scientifically defendable approaches to accurately determine the extent of gas migration and the rates of fugitive methane emissions in the vicinity of wells. Therefore, the objective of this project is to test new approaches to determine the extent of fugitive gas (e.g. CH_4 and CO_2) emissions around well casings.

Research strategy

The research approach is to determine the soil gas baseline conditions at the Containment and Monitoring Institute's (CaMI) Field Research Site near Brooks, Alberta, and to identify the extent of potential gas migration around well installations at the site. This is achieved by determining chemical and isotopic compositions of baseline soil gases obtained from various depths and distances from the wells using field-based and laboratory-based measurement approaches. Interpretation of the obtained data reveals which processes generated soil gas CO_2 and CH_4 thereby revealing their sources and potential depth of migration.

Desired outcomes

The outcome of this project will be improved approaches to effectively determine the extent of gas migration and the rates of fugitive methane emissions, or the lack thereof, in the vicinity of wells utilized for oil and gas production from conventional and unconventional hydrocarbon reservoirs.

Fugitive methane emissions

Towards a better quantification of gas migration in the vadose zone

Dylan Riley
MSc student

Introduction

Dylan Riley's research is focused on determining the soil gas baseline conditions at the Containment and Monitoring Institute's (CaMI) Field Research Site (FRS) near Brooks, Alberta, and on potentially existing legacy gas migration. His project quantifies the chemical and isotopic compositions of baseline soil gases and infers what processes are involved in creating those baseline conditions at CaMI. This will enable future research to determine potential impacts of carbon storage and methane gas migration on vadose zone gas conditions and on greenhouse gas (GHG) emissions to the atmosphere.

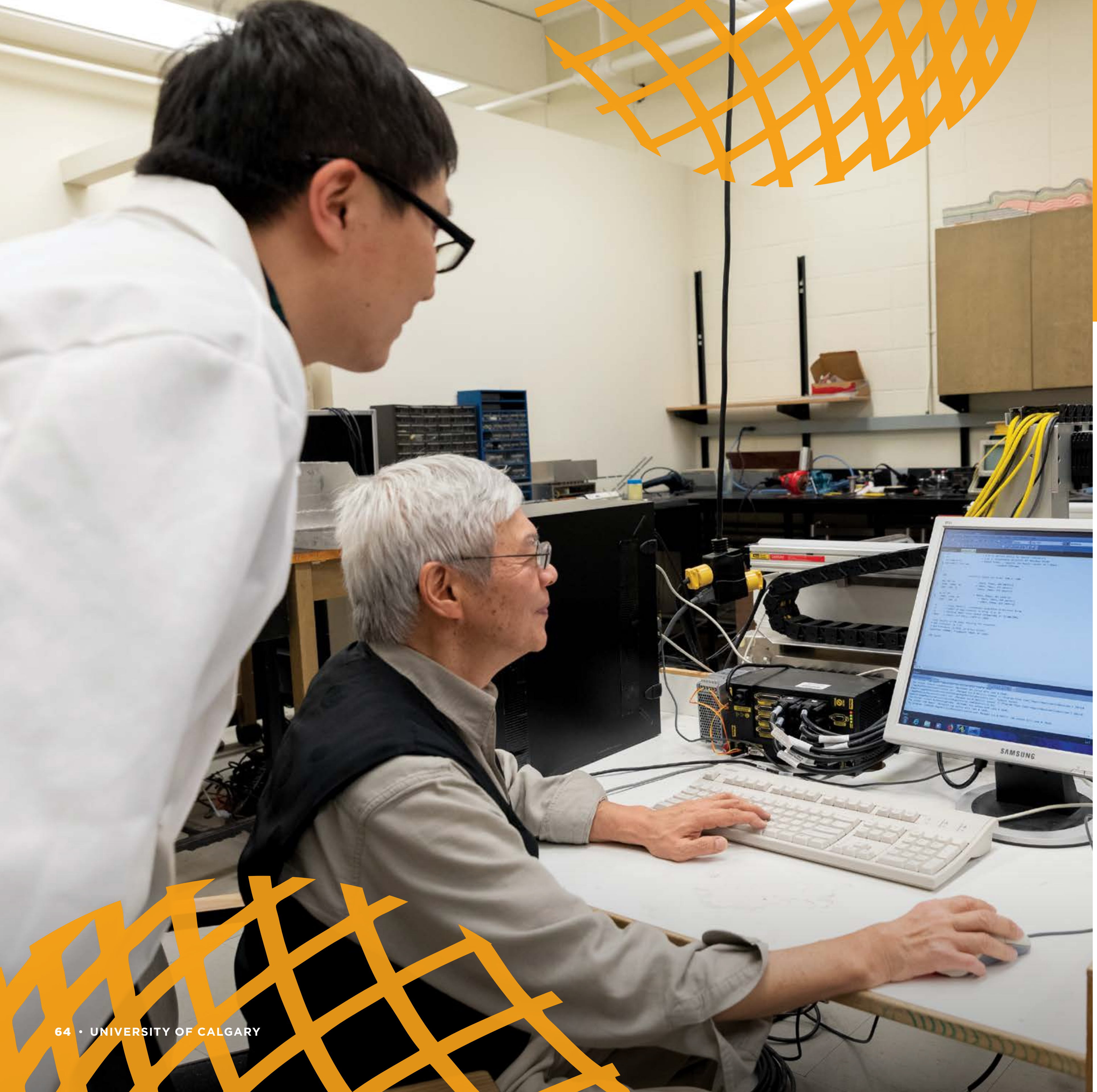
Results

Analysis of the vadose zone gas conditions at CaMI has determined that methane gas migration is not presently occurring around legacy infrastructure and is not significant around recently installed modern (post-2015) research infrastructure. However, a minor surface casing vent flow was identified at the geophysical monitoring well. Gas chromatography and mass spectroscopy work revealed that the soil gas is predominantly composed of nitrogen and oxygen, with low levels of CO_2. CO_2 concentrations are low due to the dry and compact nature of the soil and the corresponding reduced plant and biological activity in the soil. Using a fixed gas ratio of nitrogen, oxygen, CO_2 and isotopic tracers, it appears that CO_2 is predominantly sourced from respiration, calcite dissolution and methane oxidation.

Conclusions

Gas migration is insignificant around legacy infrastructure and the recently installed (post-2015) modern research infrastructure at baseline conditions.

The obtained knowledge of sources and occurrence of CO_2 and methane in soil gases at the CaMI FRS will be highly valuable for tracing CO_2 and methane leakage through the vadose zone and into the atmosphere, once CO_2 injection commences at the site.



IMPROVED RESERVOIR CHARACTERIZATION BY ADVANCED SEISMIC PROCESSING

Kristopher Innanen

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 as 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 also basic scientific value.

Improved reservoir characterization by advanced seismic processing

Raul Jose Cova Gamero
Postdoctoral Fellow

Introduction

The goal of this project is to test and develop processing workflows and algorithms for conditioning land seismic data prior to full waveform inversion (FWI) processing. The challenges in this area include proper handling of near-surface effects, presence of strong elastic effects, lack of low frequencies and poor signal-to-noise ratio. The effects of each of these features on the FWI output need to be understood to mitigate their footprint on the resulting Earth models.Due to the high computational cost of the FWI process, the research team is required to use high performance computers to execute the workflows over field data sets. This also impacts the deployment and design of the workflows and algorithms.

Results

A raypath-consistent processing workflow was developed for removing near-surface travel time effects from converted-wave seismic data. Figure 1 shows the results of computing a common-receiver stacked section with a conventional solution (top) and a raypath-consistent solution (bottom). The raypath-consistent solution provided a seismic image with more coherent and continuous events especially in the shallow (less than 1 second) part of the section. A set of forward modelling and FWI algorithms were edited and conditioned for deployment in the Compute Canada super computer. The inversion codes were rigorously tested using synthetic datasets with different acquisition configurations and optimization options (Figure 2). Results show that inverting multicomponent data using a limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) optimization provided inverted models with minimum crosstalk effects. A vertical seismic profile with a walk-away configuration provided by Devon Energy was processed. Figure 3 shows the input raw data (left) and the processed data (right) with their corresponding frequency spectrum. Tube waves and random noise were successfully attenuated. No significant raypath-dependent near-surface effects were identified on the Devon dataset. Figure 4 shows that the near-surface corrections for the shallowest (2302.7 meter depth) and the deepest receiver (3445.6 meter depth) differ in average by ±1 millisecond. Therefore, a conventional elevation static correction was implemented. The inversion of these data after using different pre-processing strategies is still a work in progress.

Conclusions

Raypath-consistent corrections provide a better approximation for removing near- surface effects from shallow events without compromising the image quality at larger depths.

However, for acquisition configurations with limited depth coverage raypath-dependent effects are difficult to identify and a conventional surface-consistent correction might suffice.

Land seismic data demand pre-processing strategies to account for the missing physics on the FWI scheme being implemented.

These strategies not only depend on the FWI algorithm but also on the data acquisition configuration.

Dr. Raul Jose Cova Gamero, PhD, acknowledges Compute Canada for their assistance.

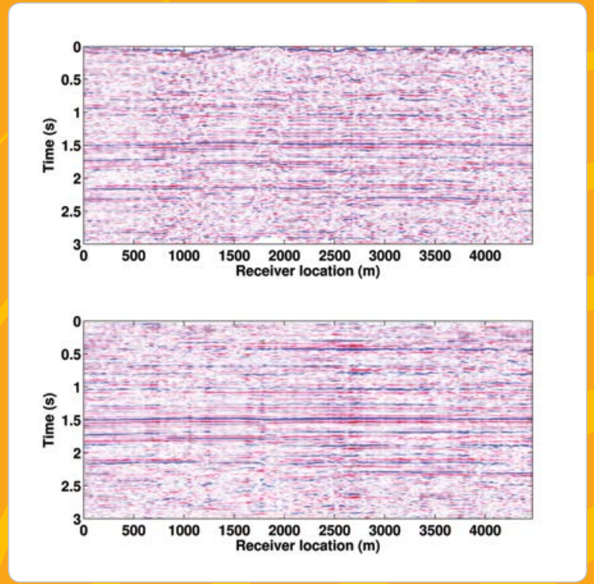


Figure 1

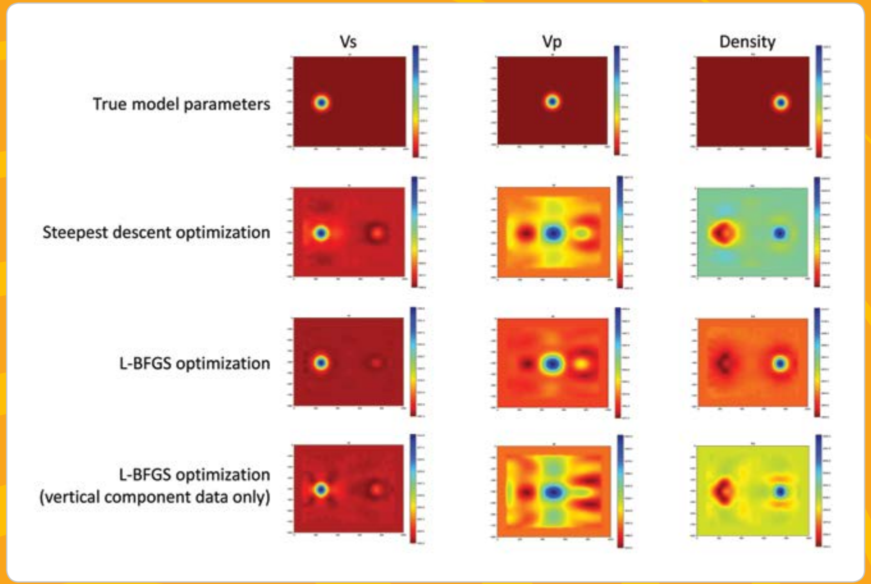


Figure 2

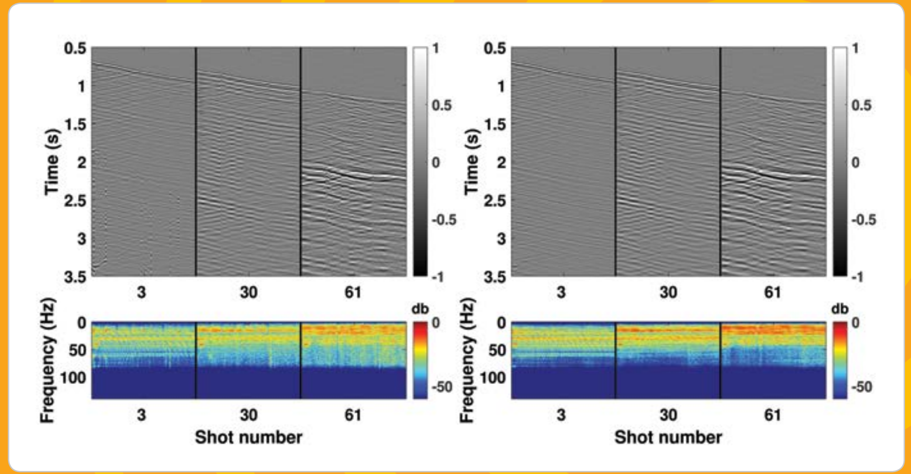


Figure 3

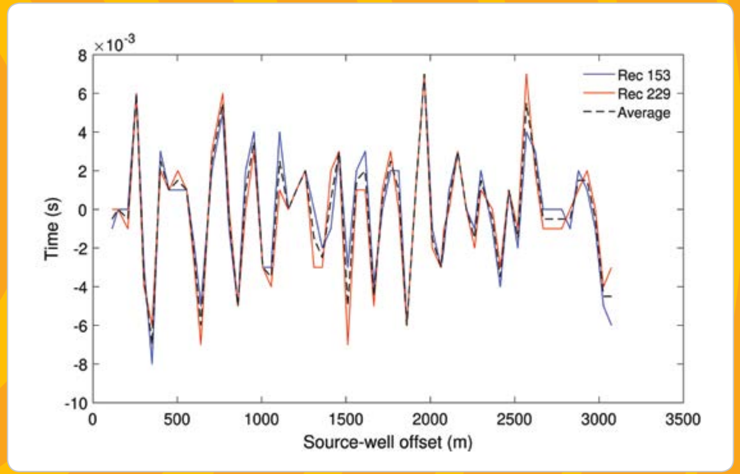


Figure 4

THEME 3: CO_2 CONVERSION

The Theme 3 research group led by Dr. Marc Strous, PhD, is engaged in developing processes for CO_2 conversion and sequestration, as well as for producing hydrogen or electricity from petroleum reservoirs. The research 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. The 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 microbial fuel cells or flow batteries, with electrodes placed inside the reservoir or electron shuttles recycled between the reservoir and an above ground fuel cell.

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. Viola Birss, Steven Bryant, Ian Gates, Kunal Karan, Steve Larter, Warren Piers, Edward (Ted) Roberts, George Shimizu, Venkataraman Thangadurai, Joule Bergerson, Roland Roesler, Roman Shor, Hector De la Hoz Siegler, Sathish Ponnurangam, Jeffrey Van Humbeck and Gregory Welch.

SYZYGY: ZERO CO_2 EMISSION ENERGY EXTRACTION FROM PETROLEUM RESERVOIRS

Steve Larter, Venkataraman Thangadurai, Marc Strous, Steven Bryant, Joule Bergerson, Roman Shor

Other participants: Kunal Karan, Edward (Ted) Roberts, Ian Gates

Background

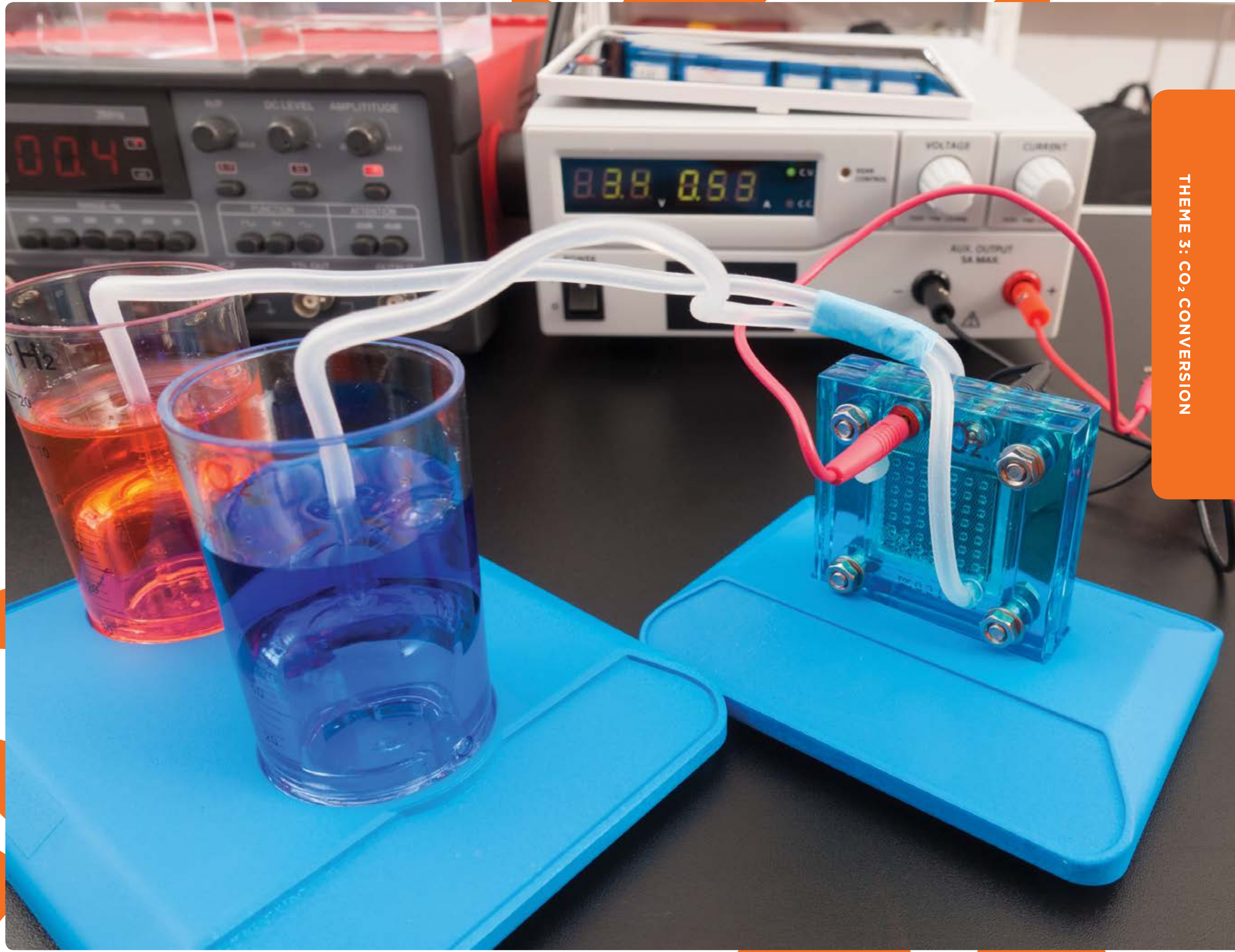
Combustion of fossil fuels and the resulting CO_2 emissions is the major source of global warming and other environmental concerns today. One global challenge involves transitioning energy systems away from fossil fuels to large-scale renewable energy systems. Part of this transition could include zero carbon energy derived from fossil fuels by radically new technologies. The SYZYGY project will assess processes and develop pilot systems for evaluation. Technologies should be capable of recovering zero carbon energy from petroleum reservoirs at equivalent rates to oil and gas energy recovery.

Research strategy

In this project, researchers seek technologies that permit zero emission energy, recovered and used, from fossil fuel reservoirs, oil and gas or coal. They focus on the feasibility of direct electrical power generation from fossil fuel reservoirs specifically through biologically mediated processes. Several routes to zero emission energy recovery have been proposed from fossil fuel deposits via energy vectors, such as hydrogen, ammonia and electricity. These dissect into two groups of processes: (1) conversion processes that convert the fossil fuel resource into a surface transportable zero carbon energy vector material such as hydrogen or ammonia and (2) direct production of electricity from the reservoir resource using electron transporters such as electron shuttles or electrons themselves. These processes are termed transporter processes. SYZYGY is currently pursuing two technology families. The first uses electron shuttles such as metal ions, which were circulated to the reservoir where microbes use them to oxidize crude oil, the reduced shuttles being produced to the surface where they enter a fuel cell and generate electricity before being recycled to the reservoir. The second route looks at the feasibility of direct electrical power production from the reservoir using microbial fuel cells.

Desired outcomes

If practical electrical power generation from fossil fuel reservoirs could be achieved at significant scale this would prove to be a revolutionary achievement, both for the transition of the oil and gas industry and also for society. It would encourage the oil and gas industry to assist in development of electrochemical renewable energy systems and permit large fractions of Canada's currently stranded oil and gas resources to be developed and used, in a truly zero emission, cleantech manner.



SYZYGY: Zero CO_2 emission energy extraction from petroleum reservoirs

Direct production of electricity from oil fields using electron shuttle systems

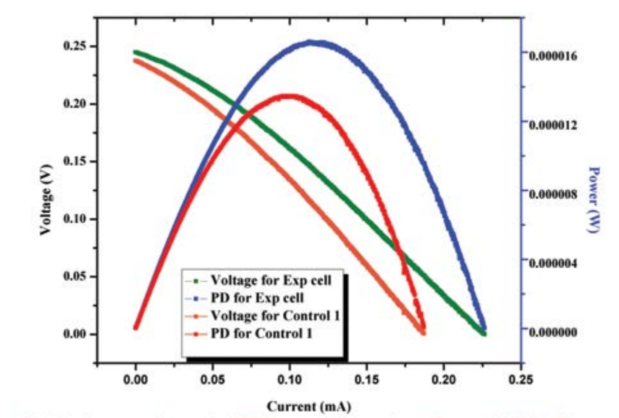
Arpita Nandy
Postdoctoral Fellow

Introduction

The main focus of Dr. Arpita Nandy's research, is direct electricity production from oil fields using microbial fuel cell (MFC) technology. The basic idea is to use the organic components of crude oil for microbial oxidation and generation of electrical energy, simply converting the chemical energy of oil into electrical energy by microbial catalysis. The process can be further accelerated with the aid of electroactive shuttles. The idea is unique, yet it is challenging to achieve optimum operational parameters for a practically viable system. The technique is sustainable to biologically utilize oil organics in a cost-effective manner with the additional advantage of generating "clean energy".

Results

A biological fuel cell is different from a chemical fuel cell despite their similar working principle. A biological fuel cell is limited by the magnitude of power derivable as well as by the constructional and operational challenges. It can be a preferable choice for its sustainability and lesser carbon footprint on nature. So far, Dr. Arpita Nandy, PhD, has been able to generate power in the low range (around 50 milliwatt per square meter) using a low concentration of crude oil together with bacterial growth media. While this value is in the range of what is expected from a typical MFC, there are still many parameters to work on for improving the performance. The main challenge now is to achieve stable, easy to maintain, efficient systems operating in more realistic conditions (i.e. a higher percentage of oil). Arpita is working towards optimizing the complex and diverse parameters influencing the performance of MFC directly or indirectly.



Polarization curve for a typical MFC generating maximum Power of 0.016 mW

Conclusions

This project is exciting yet challenging and initial results show a promising prospect.

Process optimizations would be a major component to establish a stable and efficient system.

Arpita is looking forward to addressing the technical and operational challenges associated with her project.

SYZYGY: Zero CO_2 emission energy extraction from petroleum reservoirs

Breda Novotnik
Postdoctoral Fellow

Introduction

The project's aim is to evaluate the production of green electricity from crude oil via microbial transformations. The research of Dr. Breda Novotnik, PhD, focuses on coupling microbiological anaerobic crude oil consumption with a solid metal oxide or organic compound reduction. Further re-oxidation of these reduced species would lead to electricity generation. Such microbiological processes are currently unknown especially in natural samples, where mixed microbial communities are present. Due to the complexity of microbial processes in these natural samples and the extremely slow nature of anaerobic crude oil oxidation, Breda has also been working on metal reduction providing microbes with easier to digest substrates such as lactate.

Results

Breda has tested various natural samples as sources of microbial communities. She has also examined several carbon sources and different metal oxides as electron acceptors. Almost 150 different combinations of electron acceptors, donors and microbial sources have been tested and most of them have not demonstrated microbial activity. Breda and her team are now focusing on manganese oxide, specifically birnessite (Figure 1), and anthraquinone-2-sulfonate reduction with crude oil oxidation by microbes from activated sludge. Additionally, she has been studying metal reduction with lactate as a carbon source in these systems instead of crude oil (Figure 2). These experiments have shown that microbial fermentation is a surprisingly important process despite the presence of even surplus electron acceptors. To prove that fermentation of substrate as well as metal reduction are important when crude oil is the sole carbon source, Breda is currently conducting enriched ^{13}C (carbon isotope) hexadecane and naphthalene experiments and recording delta ^{13}C measurement of CO_2.

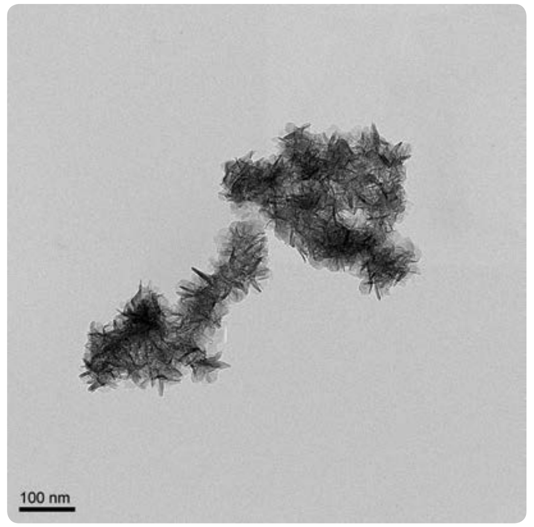


Figure 1

Figure 2

Conclusions

Breda performs microbial anaerobic crude oil oxidation as well as a dissimilatory metal reduction in her experiments.

Despite the presence of electron acceptors, fermentation of easily degraded as well as complex carbon sources is an important process.

Fermentative microbial organisms dominate within the microbial population, with metal-reducing bacteria presenting only a small fraction of the population.

Alternative vectors for carbon storage (AVECS)

Calista Yim
MSc student

Introduction

Calista Yim works on storing atmospheric carbon as biologically refractory water-soluble organic molecules into shallow saline aquifers that have been contaminated. Her first approach is to convert organic waste material to biodegradation-resistant and water-soluble inert carbon using sulfurization and oxidation reactions. To understand the chemistry of refractory species, Calista has been examining high sulfur content oil fractions. She has been concentrating sulfur-rich fractions from oils, as model systems, then oxidizing the fraction to create model carbon-rich water-soluble fractions. Calista's aim is to develop a cost-effective carbon storage method that is globally accessible and as impactful as sulfur using abundant resources, like contaminated aquifers. Some challenges include method development and long experimental times.

Results

Lipid sulfurization results show 2-4 sulfur atoms are incorporated into lipids structures, which means compounds are potentially more biodegradation-resistant compared to their original forms. Estimation Programs Interface (EPI) Suite BIOWIN software has an estimated biodegradation rate of compounds and shows sulfurized lipids are recalcitrant, whereas the original lipids biodegrade in a few weeks to months. Furthermore, EPI Suite WATERNT software indicates water solubility is improved 50 times when sulfurized products are oxidized. Oxidation reactions will be investigated in future work. As for extracting sulfur-rich fractions, Calista is working on adjusting the extraction method. Liquid chromatography methods in literature use baked silver nitrate mixed with silica gel, however, this does not work in the dry Calgary climate because the silica gel becomes very reactive and retain most of the components including the desired sulfur-rich fraction. Therefore Calista is currently adjusting the method to obtain the sulfur-rich fraction.

Conclusions

Organic compounds with chemical structures such as double bonds, carbonyl groups and hydroxyl groups are more likely to incorporate sulfur atoms into their structure.

Sulfurization reactions have been successful and improve biodegradation resistance.

Sulfurization experiments using heat and carbohydrates are currently being examined.

Sulfur compound fractionation procedures are being developed.

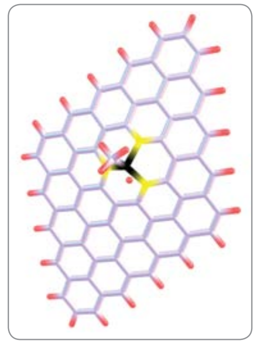
SYZYGY: Zero CO_2 emission energy extraction from petroleum reservoirs

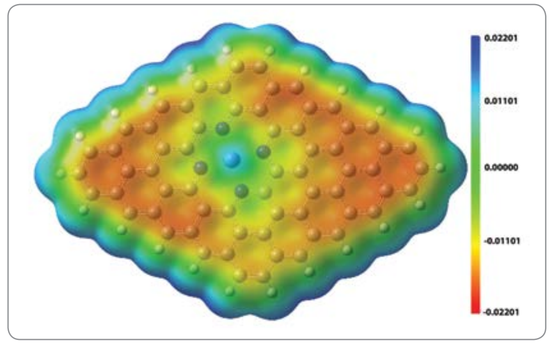
Computational study on methane activation and CO_2 reduction

Chongchong Wu
Postdoctoral Fellow

Introduction

The research of Dr. Chongchong Wu, PhD, regards the conversion of the greenhouse gases CH_4 and CO_2. The challenges for CH_4 activation and CO_2 reduction are that CH_4 and CO_2 are quite stable, and existing catalysts are too expensive. Chongchong's project is to design efficient and cost-effective catalysts for CH_4 activation and CO_2 reduction. The research will reduce greenhouse gases and at the same time, produce valuable chemicals from these greenhouse gases.





Results

The main outcome of the research is that a cheap single atom catalyst (SAC) has been designed for CH_4 activation positioned on graphene. In addition, the research has led to an effective catalyst for CO_2 reduction. Chonchong faced some failures during simulation. Since these catalysts have so many electrons, the optimized structures could not be obtained easily. Sometimes, over 50 tries were made to obtain the most stable structures and transition states, however this has been a great learning for her.

Conclusions

- Vacancy sites on graphene influences the catalytic activity of SAC.
- Single iron atom on single vacancy graphene with three doped nitrogen has a low energy barrier for methane activation.
- SAC doped on molybdenum disulfide (MoS_2) promotes the catalytic reduction of CO_2.

SYZYGY: Zero CO_2 emission energy extraction from petroleum reservoirs

Tuning optoelectronic properties of PEDOT: PSS ultra thin films for electrochemical and other applications

Ehsan Hosseini
PhD student

Introduction

The electrodes of electrochemical devices must provide facile electro-conduction. Conducting polymers such as polymer poly (3, 4-ethylenedioxythiophene): poly(styrenesulfonic acid) known as PEDOT: PSS is a relatively new material class that can provide such functionality. This project involves tuning the properties of PEDOT: PSS and its nanocomposite, made with additives such as graphene or metal nanowires, for electrochemical applications. Transparency of these polymers is required for solar-based devices. Ehsan's goal in this project is to attain sufficiently high electron conductivity and optical transparency for PEDOT: PSS based materials.

Results

Ehsan aims to attain a very high conductivity and transparency of PEDOT: PSS based materials via a specific solvent treatment process. Interestingly, his team has discovered a reasonably good electromagnetic shielding property in the process of electrical characterization of this material, which has opened up avenues for new applications. The team is currently in discussion about invention disclosure and the possibility of filing a patent. Unexpectedly, Ehsan has encountered negative results wherein the material degrades after certain treatment processes. However, through infrared spectroscopy measurements, he has been able to identify the mechanism of the degradation. So far, new results sufficient for two manuscripts have been generated. Experiments are ongoing to enhance the aforementioned properties even more to meet the requirements for the electrochemical and other applications.

Conclusions

- Ehsan has generated highly conductive and transparent polymeric films using solvent treatment methods.
- He has fabricated films with noticeable electromagnetic interference shielding effectiveness above 20 decibels for the applications where transparency plays a key role.
- He is currently investigating the doping of PEDOT: PSS with different fillers to make nanocomposites.

SYZYGY: Zero CO_2 emission energy extraction from petroleum reservoirs

Jagos Radovic
Postdoctoral Associate

Introduction

Dr. Jagos Radovic, PhD, and his team are working on a technology to extract electrical energy from fossil fuel deposits. It is based on below-ground microbial oxidation of oil or bitumen, retaining the CO_2 below ground and capturing biogeochemical energy in the form of a transportable, reduced electron shuttle (e.g. manganese, iron, quinones). The reduced shuttle is then recovered and re-oxidized above ground, coupled with the production of electricity. Challenges are flow rate restrictions, maximum viable shuttle concentrations, reservoir damage issues, etc. Impact of this project is game-changing — it would enable the use of Canada's natural fossil fuel resource, without CO_2 emissions to the atmosphere.

Results

The main results of this project to date include the detection and quantification of hydrocarbon degradation in the model microcosms containing model electron shuttle (manganese and iron oxide) and oil, both within saturated and aromatic fractions; with character trends for biodegradation (e.g. less degradation with increasing alkylation, C_{17}/pristane, C_{18}/phytane ratios, etc.). In addition, Jagos has been able to detect oxidized chemical species (e.g. phenols, acids) after incubation with electron shuttles — putative degradation intermediates/products of oil biodegradation. Chemical characterization studies are conducted in parallel with the microbial community structure analyses, to demonstrate the coupling of microbial oil degradation to electron shuttle reduction, as well as electrochemical studies of the candidate redox active species.

Conclusions

Jagos and his team have obtained promising results which seem to validate the main concepts of the proposed technology, (i.e. microbial hydrocarbon degradation and electron shuttle reduction, and the reversible redox activity of candidate electron shuttles).

Other spin-off technologies are emerging (e.g. for pollutant remediation and novel, organic-based redox flow systems).

SYZYGY: Zero CO_2 emission energy extraction from petroleum reservoirs

Renzo Correa Silva
Research Associate

Introduction

Sequestering the vast amount of atmospheric material that is required to limit global climate change impacts is an outstanding issue, mainly because CO_2 underground storage is expensive and geographically restricted. The Alternative Vectors for Carbon Storage (AVECS) research project addresses this issue by developing affordable and sustainable routes for carbon storage in geological settings. Such an approach is an innovative negative CO_2 emission strategy that, if successful, stands poised to immediately revolutionize carbon storage technologies and mitigate pollutant loads associated with petroleum extraction.

Results

In the lab, Dr. Renzo Correa Silva, PhD, and his team have explored new routes for waste biomass modification (mainly cellulose and lignin), although the targeted water solubility of obtained products is still one order of magnitude short of the ultimate project goals. Experiments, where sulfur is tested as the key ingredient for waste biomass alterations, are still ongoing, and the investigation of the natural sulfurization of sedimentary organic matter has given important insights to potential cost-effective routes.

Conclusions

Early results are encouraging. Renzo and his research team have made the most out of the resources available, but there is still much work to be accomplished.

SYZYGY: Zero CO_2 emission energy extraction from petroleum reservoirs

Senthil Velan Venkatesan
Postdoctoral Fellow

Introduction

Dr. Senthil Velan Venkatesan, PhD, is developing an energy conversion device compatible with oil reservoirs. The bioactivity in oil reservoirs is exploited in electrochemical energy conversion. The major challenges in the project include the design of the device, electrolytes involved, constraints on the concentration of redox active material, optimization of the device for field application, scalability and durability. Senthil has been attempting to construct a prototype device for oil reservoir with anode and cathode in separate compartments similar to an electrolyzer. This design, if realized, can be adopted in power generation with no or low carbon emission.

Results

Senthil has worked on the initial designs for redox energy conversion based on available literature. After careful iterations, he has developed a design with auxiliary electrodes connecting the anode and cathode chambers (Figure 1). He has identified required materials through basic electrochemical and material studies. Senthil has constructed a single-cell using vanadium, organic and metal complex redox couples and has studied their half cell/full cell and charge/discharge properties. Senthil's four-cell prototype using auxiliary electrode design has been able to light an LED lamp for a few seconds. The current drawn from the cell is limited to a few microamps and self-discharge of the cell is significant. Hence, Senthil and his team are investigating paths to increase the current drawn from the cells by maximizing electrode area and electrolyte concentration. He is planning to build a prototype using iron-air in redox cell. He plans to have a better understanding of redox chemistries of electrolytes and auxiliary electrodes via fundamental material studies.

Conclusions

- Senthil has demonstrated the feasibility of separate compartment redox cells in alkaline and acidic electrolytes.
- The electrochemical characteristics of the separate compartment redox cells are similar to the conventional redox flow batteries.
- Redox function of auxiliary electrodes facilitates the ion-electron-ion transfer across anode and cathode chambers.
- Senthil's six volt prototype is shown in Figure 2 and the charge/discharge behavior is presented (Figure 3).

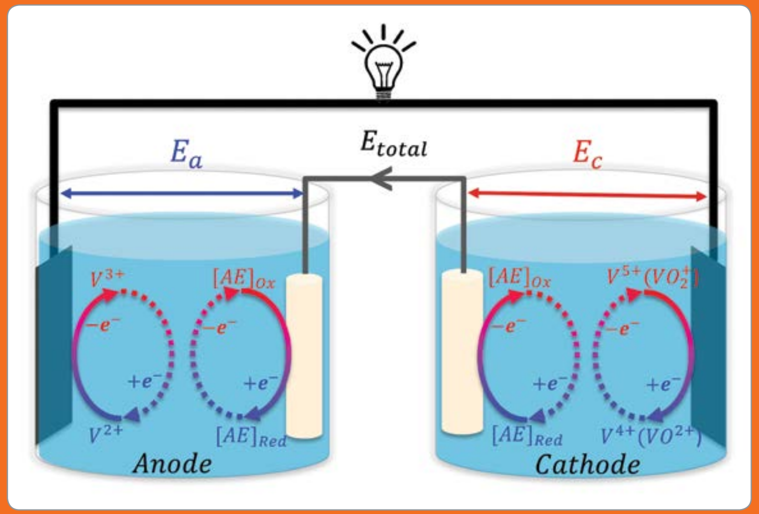


Figure 1

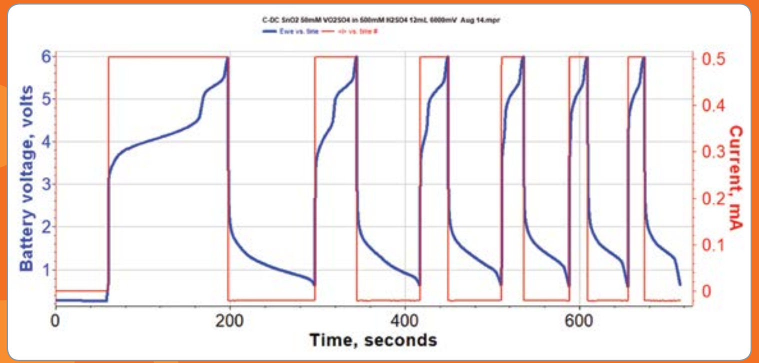


Figure 3

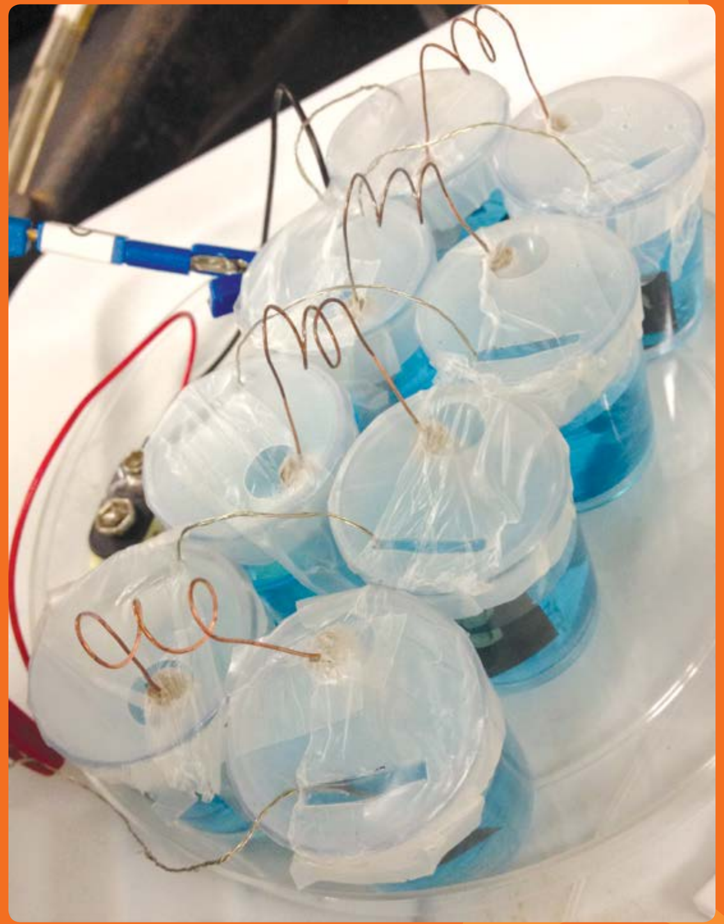


Figure 2

CAN EFFICIENT, COST-EFFECTIVE CO_2 REDUCTION CATALYSTS BE DEVELOPED? (SYNTHETIC FUELS)

Warren Piers, Viola Birss, Gregory Welch, Kunal Karan,
Roland Roesler, Sathish Ponnurangam

Background

One of the most promising strategies for the development of more carbon-neutral fuels is the reduction of CO_2 to CO, and from there to liquid fuels (higher hydrocarbons) via the Fischer-Tropsch process. Provided the energy needed to drive the CO_2 reduction (and H_2 production) is derived from renewable sources, and the CO_2 employed is taken from the atmosphere, a near carbon neutral cycle is established. For this process to be feasible, new catalysts are required that accomplish this conversion with high selectivity, the right balance between activity and longevity, low cost and scalability. A promising and underexplored strategy is to develop hybrid systems by depositing promising catalyst classes on novel nanostructured and conducting supports.

Research strategy

In this project, Prof. Warren Piers and his research group are targeting such hybrid catalysts with the aim of discovering selective, long-lived catalysts for CO_2 conversion to CO. They will synthesize molecular electrocatalysts with appropriate functional groups and develop methodologies to affix them to novel support materials. Full characterization of these hybrid catalysts using modern surface characterization techniques and evaluation of their catalytic behavior in comparison to the molecular species will be done. Another strategy would be nanostructuring the catalyst layer primarily to increase catalytic area (e.g. producing nanotubular oxide structures and infiltration of catalytic nanoparticles into catalyst scaffolds).

Desired outcomes

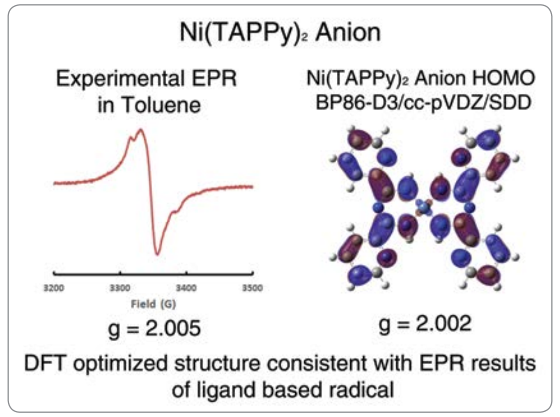
The current and planned research aims at the synthesis and benchmarking of 2-3 families of molecular CO_2 reduction catalysts; synthesis of functionalized CO_2 reduction catalysts for supporting on porous carbon and other nanostructured conductive supports; development of methods for characterizing these supported hybrid catalysts and evaluating their performance as CO_2 reduction catalysts; achieving improved perovskite catalyst performance, potentially also at lower temperatures, through novel nanostructuring and compositing approaches; development of novel characterization tools to better understand the performance of existing heterogeneous catalysts and to then knowledgeably transition towards new generation materials; integration of catalysts into prototype devices for CO_2 reduction.

Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Alexander Hyla
Postdoctoral Fellow

Introduction

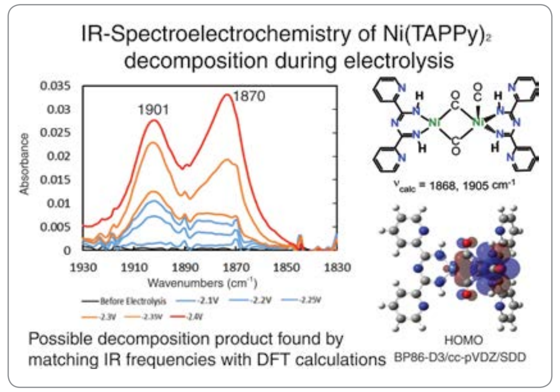
Dr. Alexander Hyla, PhD, is investigating how to model new electrocatalysts for CO_2 reduction to products that can be used to create fuels, such as CO. He is obtaining energy levels and redox potentials of these new catalysts using density functional theory (DFT). Alexander's team is studying new ligand frameworks that have potential to be electrocatalysts, but the extent of their catalytic activity is not known until tested.
The team is trying to understand the mechanism of catalysis both through experimental and computational results. This work will add to the wealth of knowledge in the literature and has the potential to influence future investigations into CO_2 reduction.



Results

Alexander has been modelling the TAPPy (1,3,5-triazapentadienyl-2,4-bis(2-pyridyl)) ligand for CO_2 electroreduction. He has been studying the effects of solvation, modification of the ligand framework with electron-donating and electron-withdrawing groups, and changing the central metal atom in the catalyst, which has the general form $M^{II}(TAPPy)_2$. He has also been examining the decomposition products, wherein, the nickel (Ni) version of the catalyst decomposes under electrolysis conditions. He has been able to predict infrared active frequencies for a potential decomposition product that matches infrared-spectroelectrochemistry results, suggesting that this product is created during electrolysis. Alexander's team is currently compiling data and writing a draft for communicating the results.

Additionally, now that the TAPPy project is near conclusion, Alexander is looking into other ligands, which includes porphyrin-like macrocycles with imidazole and pyridine components. For this, he is comparing energy levels and redox potentials to known catalysts to determine if these catalysts should be prepared and tested.



Conclusions

- First and second one-electron reductions of $Ni(TAPPy)_2$ are almost exclusively ligands based.
- $Ni(TAPPy)_2$ decomposes under electrolysis conditions.
- $Ni(TAPPy)_2$ under electrolysis conditions likely creates $(NiTAPPy)_2(\mu\text{-}CO)_3$ due to infrared frequency matching.

Dr. Alexander Hyla, PhD, acknowledges Compute Canada and the High-Performance Computing group, University of Calgary for computational resources.

Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Amir Alihosseinzadeh
PhD student

Introduction

The electroreduction of CO_2 (CO_2RR) to chemicals such as CO shows great potential for renewable fuel and chemicals production. In this project, Amir Alihosseinzadeh's focus is to develop a new catalyst with high selectivity towards the formation of hydrocarbons and multi-carbon oxygenates at high efficiencies and good stability. Among different catalysts screened for CO_2 reduction, transition metals like copper exhibit a high selectivity towards formation of hydrocarbons and multi-carbon oxygenates at fairly high efficiencies. Also, carbon-based structures with a high surface area, low cost, and significant electrocatalytic activity provide an appropriate substrate for active transition metals for the CO_2RR.

Results

Through literature review, Amir has learnt about the reported performance of a wide range of transition metal catalysts, metal-free catalysts, and carbon-based materials for the CO_2RR. He has been able to evaluate the catalytic performance of catalysts and design an H-cell. Also, he has set up a test-station system for the catalysis evaluation under continuous feed stream. He has redesigned an existing gas chromatograph, calibrated, and benchmarked to analyze the products of the catalytic reaction including an appropriate configuration with a specific column and detectors. Amir has analyzed a variety of methods for the synthesis of graphene-based catalysts and is presently studying various levels of doping and metal nanoparticles incorporation. Next, he is testing the synthesized catalysts for their electrochemical properties (e.g. cyclic and linear sweep voltammetry).

Conclusions

- Amir has been able to identify the critical gaps that prevent commercialization of this technology using traditional metal-based heterogeneous electrocatalysts.
- He has implemented a new design using an Agilent GC to perfectly suit the analytical process.
- He has set up an H-cell and test stations which are being benchmarked. The synthesized catalysts are being evaluated under batch and continuous modes in these cells.
- He has fabricated graphene-based catalysts with nitrogen, boron, and copper doping.
- Amir has trained for atomic force microscopy (AFM), scanning electron microscope (SEM) and nuclear magnetic resonance (NMR) spectroscopy techniques.

Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Synthesis and development of earth-abundant metal catalysts for the electrochemical reduction of CO_2

Braulio Puerta Lombardi
MSc student

Introduction

Braulio Puerta Lombardi works on developing catalysts that are highly active on the conversion of CO_2 into more useful materials. The former is a gas widely produced in the combustion of fossil fuels, making its use as a feedstock chemical an attractive prospect. However, this transformation is not an easy feat, and the reduction of the energy required by this process is paramount. A select number of reported transition-metal complexes have been shown to catalyze the electrochemical conversion of CO_2 into carbon monoxide, formate, and oxalate. Learning from these examples, Braulio's team has been developing catalysts based on earth-abundant, low-cost metals using rational design.

Results

Braulio has started the research by synthesizing a target pentadentate nickel complex which contains many features deemed crucial for the development of a high-performing catalyst. However, molecular stability issues and low product yields have redirected the team to a different target (also nickel-based). The latter can be achieved in merely two synthetic steps and preliminary results have shown promising activity towards CO_2 electroreduction. Based on these initial results, Braulio has focused on expanding the scope to other earth-abundant metals (iron, cobalt, zinc) and in testing the catalytic performance of various derivatives. Although the metrics ultimately has turned out to be sub-optimal, a substantial amount of insight has been gained on the catalyst system in terms of its molecular properties and mode of operation, which has proven essential for surveying potential future candidates. Furthermore, the work done thus far will be published in a peer-reviewed journal.

Conclusions

- Braulio has developed a derivative of the main synthetic target to better understand the properties of the system under study by his colleagues.
- His findings have been the key to understanding the synthetic strategies and characterization techniques essential for producing a high-performance catalyst.

Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Designing molecular electrocatalysts for the conversion of CO_2 to fuels

Demyan Prokopchuk
Postdoctoral Fellow

Introduction

The electrochemical reduction of CO_2 receives continuing interest in producing chemical fuels, one carbon (C-1) synthetic building blocks and mitigating greenhouse gas emissions. Molecular electrocatalysts offer fine synthetic control in designing molecules that are active and selective for converting CO_2 to fuels. The challenge is to synthesize new electrocatalysts using abundant metals, with the final goal of implementing them in a fuel cell device for generating fuels derived from CO_2.

Results

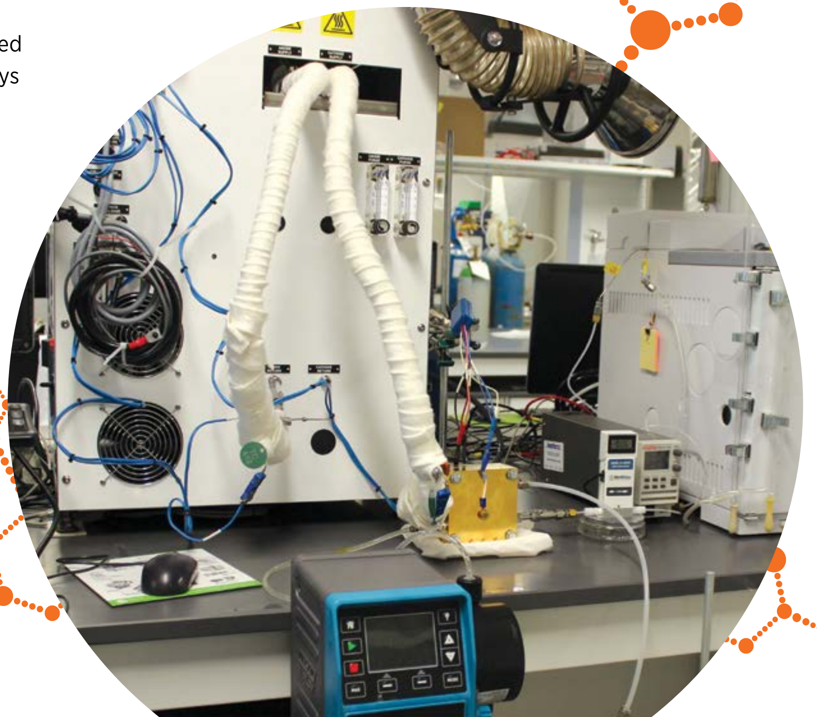
In the first set of molecular design iterations, Demyan and his team have developed a new nickel compound that reduces CO_2 to CO (a fuel precursor) in an electrochemical cell. Unfortunately, the system is not electrocatalytic. Demyan then focused his attention on why this nickel compound would not operate as an electrocatalyst. His results show that the organic framework around the nickel atom is not stable for prolonged periods of time.

Conclusions

Demyan and his team have synthesized new electroactive nickel molecules.

Although CO_2 can be reduced to CO (a fuel precursor), the nickel compounds used are unstable over time.

Detailed mechanistic investigations have uncovered unique deactivation pathways which will drive the future design of stable, active and robust electrocatalysts for converting CO_2 into fuels.



Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Fatemeh (Parisa) Karimi Amirkiasar
Postdoctoral Fellow

Introduction

Electrochemical reduction of CO_2 to fuels as a means of reducing carbon footprint is a subject undergoing intense study globally. For exploitation of this technology, electrochemical cells operating at a steady state is desirable. Feeding the CO_2 in the gas phase can help simplify the overall system and allows for large current densities which enable high production rates. Dr. Parisa Karimi, PhD, and her team are working on the development of gas-phase electrochemical cells for CO_2 electrolysis or CO_2 electro-reduction. The challenges related to the technology are lack of an efficient electrocatalyst that is also durable and high energy consumption in the process. Parisa is trying to engineer the electrode and membranes and incorporate existing and new electrocatalysts that exhibit low overpotential and high faradic efficiency for CO_2 reduction, and reduce the overall voltage consumption of the electrochemical cells.

Results

To date Parisa, in collaboration with her research team, has been able to complete three major tasks: (1) design and setup of gas-fed CO_2 electrochemical reactor (2) fabrication and testing of a membrane electrode assembly in a working device (3) development of protocols for electrochemical characterization of catalysts in a device.

She has been able to test silver and copper-based material in the device using a variety of different cation and anion exchange ionomers/membranes. She has achieved more than 90 per cent selectivity and 85 per cent faradaic efficiency for CO production using silver nanoparticles as the cathode electrocatalyst and anion exchange membrane/ionomer as the solid electrolyte. The current density in the current system is small and some electrode catalyst layer engineering is required to increase the current.

Parisa's research work titled "CO_2 electrolysis in solid polymer electrolyte electrochemical cells: investigating the possibility of electrolysis in gas phase" won the best poster award at an eminent, international electrochemistry conference — The International Society of Electrochemistry held in Bologna, Italy in September 2018.

Conclusions

Parisa has developed a functional gas-fed electrochemical reactor.

She has identified desirable products such as syn-gas mixture and lower hydrocarbons [acetylene (C_2H_2), CH_4] when operating in a cell with an anion exchange membrane.

Preliminary electrode engineering has shown a doubling of production rate (or current densities), however, another order of magnitude improvement is needed for attracting commercial interest.

Parisa is currently exploring new catalysts, new electrode structures and new composite membrane structures.

Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Erwan Bertin
Postdoctoral Fellow

Introduction

Dr. Erwan Bertin, PhD, is exploring various strategies to attach catalysts which have been developed by other Theme 3 research groups. These catalysts can convert the CO_2 molecule to CO at the novel 3D honeycomb carbon support materials, developed in Prof. Viola Birss' research group. The challenge here is the fact that CO_2 is a very stable molecule, so the reaction conditions to transform it are harsh. Keeping the catalyst on the support is also not straightforward. When unsupported, the organometallic catalysts investigated cannot be used for CO_2 reduction at scales pertinent to the amount of CO_2 generated by industry. If Erwan succeeds, he will be able to find a solution that will help avoid the release of tons of CO_2 into the atmosphere, thus mitigating the effect of carbon emissions on climate changes.

Results

Erwan's initial anchoring strategy has been to use diazonium chemistry to create a covalent bond with the carbon support. He has successfully anchored several probes (amino groups, ferrocene) at the surface of the 3D nanoporous scaffold (NCS), with a surface coverage between 25 and 80 per cent. However, this reaction has a poor yield. Thus, the amount of catalyst required to achieve these coverages would be prohibitively expensive. Therefore, Erwan has been investigating alternative anchoring strategies. The use of vinyl groups is promising, but still requires a significant amount of catalyst. Now, he is planning to redirect from classical, radical-based anchoring routes, towards surface confined reactions.

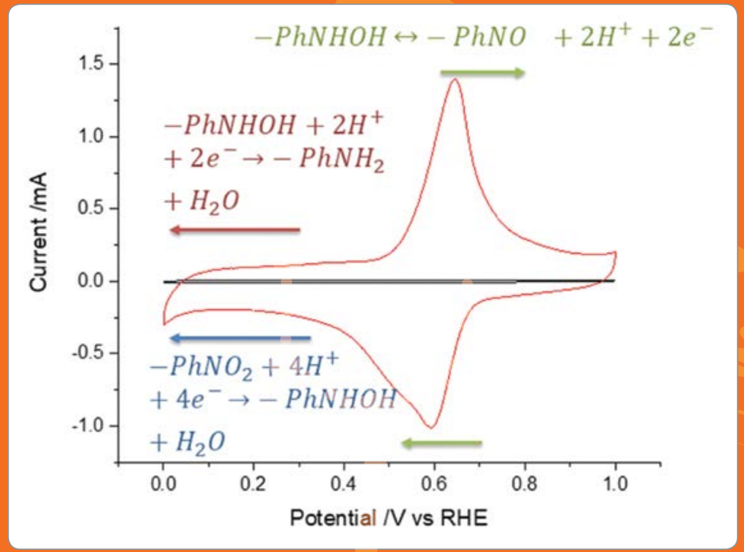
In parallel, Erwan's investigations of the nanoporous scaffold (NCS) themselves for CO_2 reduction have shown that they do have a small activity towards CO_2 reduction (about 5-25 per cent conversion efficiency). Erwan finds this interesting and is looking forward to determining what the potential active sites are at the NCS materials for this reaction.

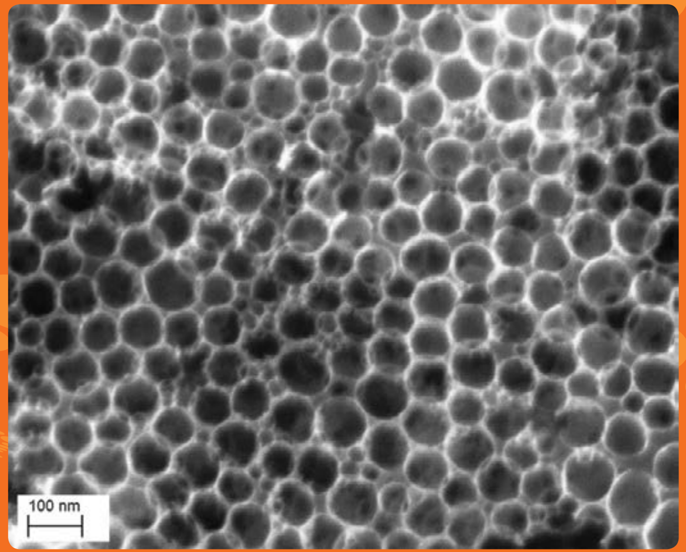
Conclusions

Diazonium chemistry successfully creates covalent bonds between a molecule and a support, reaching good surface coverages (20-81 per cent) but with low yield.

Vinyl groups also anchor catalysts on NCS, with coverage of 21-35 per cent.

The NCS material exhibits some activity towards CO_2 conversion to CO, with a conversion efficiency of between 5-25 per cent.





Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Janina Willkomm
Postdoctoral Fellow

Introduction

The goal of the project is to assemble a hybrid device for electrochemical CO_2 conversion based on molecular catalysts and nanostructured carbon supports. Creating a stable linkage between the molecular complex and a carbon material while retaining the activity of the catalyst remains one of the main challenges in the field. Better anchors and tethers have to be identified to overcome these issues. In addition, commonly used smooth carbon materials only yielded low coverage electrodes. Using nanostructured carbon supports with large surface areas enable a higher loading, and should result in a better overall performance of the device.

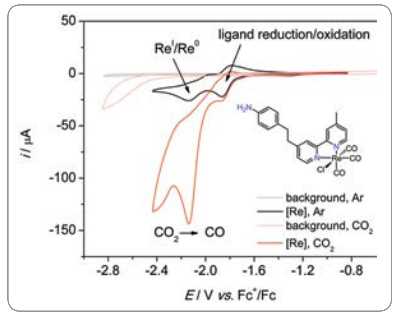


Figure 1

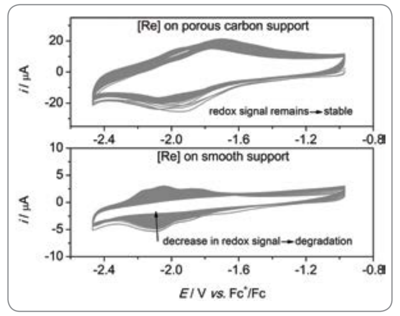
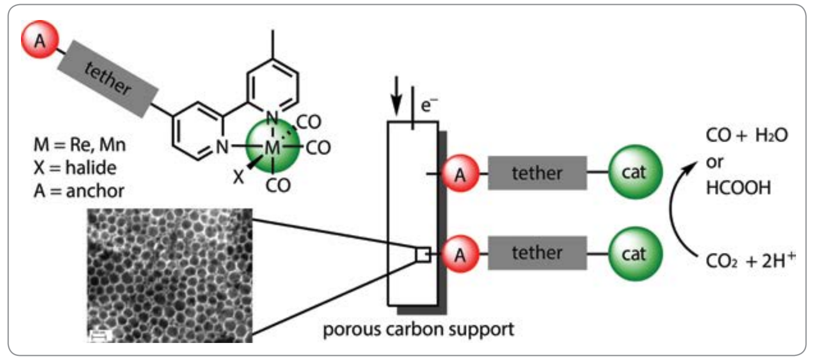


Figure 2



Results

Dr. Janina Willkomm, PhD, has modified a well-studied rhenium-based molecular CO_2 reduction catalyst on the backbone to enable anchoring to carbon surfaces via a covalent carbon-nitrogen (C-N) bond. This has kept its electrochemical activity for CO_2 conversion upon functionalization (Figure 1), and has successfully integrated with a nanoporous carbon material (provided by the Birss group) via an electrochemical grafting method. The nanoporosity does not just result in a higher loading per geometrical surface area but also stabilizes the complex in comparison to commonly used smooth supports (Figure 2). While this new hybrid electrode showed excellent stability in a moisture and oxygen-free atmosphere, it slowly degraded when tested under ambient and catalytic conditions. The reason for the instability is currently unknown and will be further investigated by advanced surface characterization techniques. Once the main cause for instability has been identified, it will be addressed to improve the linkage between the molecule and support material.

Conclusions

A modified CO_2 reduction catalyst for anchoring has been prepared.

The catalyst has been linked to a new nanoporous carbon support currently not explored in this context.

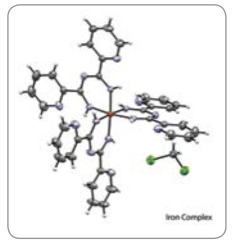
Nanoporosity improves the stability of the molecule on the surface in comparison to smooth supports.

Stability under ambient conditions needs to be improved.

Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Joshua Ethan Heidebrecht
PhD student

Synthesis and development of earth-abundant metal catalysts for the electrochemical reduction of CO_2

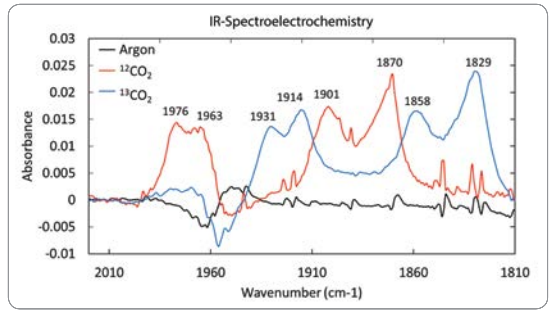


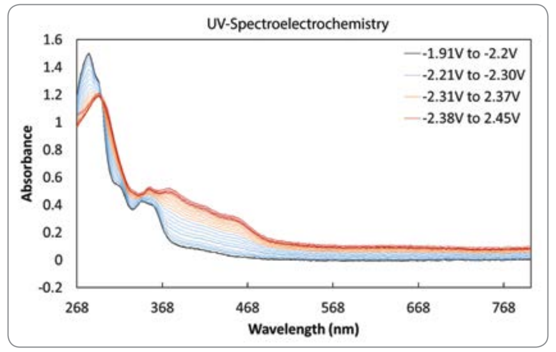
Introduction

Joshua Heidebrecht works with a multidisciplinary team targeting the conversion of CO_2, to CH_4, as a potential precursor to synthetic hydrocarbon fuels. His research focuses on the synthesis and development of catalysts employing earth-abundant transition metals for the electrochemical reduction of CO_2, tailored towards high efficiency and selectivity by utilizing recent leads in literature. 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, Joshua has worked in close proximity with graduate students in the groups of Prof. Ronald Roesler and Prof. Warren Piers towards the development of earth-abundant catalysts for the electrochemical reduction of CO_2. His extensive review of the literature has led him to the targeted synthesis of novel metal complexes incorporating an organic envelope specifically designed to enhance catalyst stability and facilitate electron transfer to the CO_2 molecule. A promising nickel-based candidate has emerged from his preliminary electrochemical testing of the aforementioned metal complexes. Following this, Joshua has spent the following months investigating the mechanism of catalysis through spectroscopic methods and has worked towards a derivative based on iron. While the results do not lead to an industrially relevant catalyst, the current manuscript in progress should provide the academic community with valuable tools towards future catalyst design and understanding possible deactivation pathways of CO_2 catalysts based on nickel.





Conclusions

Joshua has synthesized different earth-abundant metal catalysts, targeting the electrochemical reduction of CO_2.

He has identified a nickel catalyst incorporating bis(triazapentadienyl) ligands as a promising candidate.

He conducted an in-depth mechanistic study on the parent system through spectroscopic methods.

Joshua explored a derivative based on iron incorporating the same organic envelope.

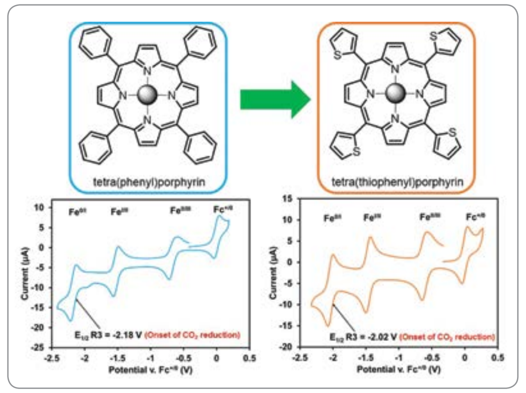
Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Bio-inspired molecules for the conversion of CO_2 to value-added products

Joshua Koenig
MSc student

Introduction

As atmospheric CO_2 levels continue to rise, it has become imperative to mitigate the associated climate effects. One promising method for diminishing atmospheric CO_2 levels is feed-stocking, whereby CO_2 is converted into value-added products through means of chemical reduction. While the electroreduction of CO_2 is quite energy intensive, it is possible to facilitate this chemical transformation through the use of molecular catalysts. Ultimately, these molecular catalysts must be designed to achieve high selectivity/efficiency, while requiring minimal energy input, when converting CO_2 into value-added products.



Results

The best class of bio-inspired molecular catalysts capable of CO_2 reduction are tetra(phenyl) porphyrins (TPP). The porphyrin scaffold can be synthetically modified quite readily through the phenyl-positions, allowing for facile tuning of chemical properties. While much research has focused on altering phenyl substituents, Joshua Koenig used his team's vast expertise in organic materials to deliver a better performing and more versatile family of catalysts based on thiophene. He has rationalized that introducing a smaller heterocycle would increase system planarity, leading to extended molecular pi-conjugation. As a result, tetra(thiophenyl) porphyrins (TThP) should become easier to reduce due to energy-level stabilization. During preliminary catalytic testing, it has been found that the newly synthesized TThP exhibits CO_2 reduction capabilities at lower overpotentials than the benchmark TPP catalyst. Research is currently ongoing to assess the efficiency and selectivity of TThP relative to TPP.

Conclusions

A new class of CO_2 reduction catalysts provides rich chemistry to tailor material properties and deliver champion performance.

Based on preliminary results, the overall energy-input required to convert CO_2 into value-added will be lower for thiophene-derived porphyrins.

Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Tethered porphyrin ligands for the electrocatalytic reduction of CO_2

Matthew Robert Wong
NSERC-USRA summer student/ research associate

Introduction

Matthew Wong has been a part of a multidisciplinary team at the University of Calgary which investigates the catalytic electroreduction of CO_2 to CO through catalysts functionalized on the carbon electrode. His research has focused on the development of earth-abundant transition metal complexes, which aims at high efficiency and selectivity for CO_2 reduction. The selectivity of the catalyst for CO_2 reduction is highly dependent on its design, as electronic and steric properties of the active site need to be tuned towards high faradaic efficiencies, stability, and low overpotentials. This will be industrially relevant as carbon monoxide is sought after in the chemical industry as a precursor to hydrocarbon fuels.

Results

During the four months of his research program, Matthew worked in close proximity with graduate students in Prof. Roland Roesler's group towards the development of earth-abundant transition metal complexes for the electrochemical reduction of CO_2. He began by synthesizing four metal complexes of the tris(pyrazolyl)methane ligand, which has then been tested for CO_2 reduction, showing no catalytic activity towards this reduction. For the majority of his term, he attempted to synthesize an organic macrocycle employing the use of two inexpensive precursors. Extensive testing of different reaction conditions to isolate the target molecule has yielded no such results that would allow the ligand to be placed on transition metals and can be tested for CO_2 reduction, although the synthesis of the target molecule has been achieved (according to mass spectrometry). Matthew then moved on to synthesize a nickel-based candidate similar to a complex found in the literature but its synthesis proved more challenging than initially thought, and this work could not be completed due to time limitations.

Conclusions

Matthew synthesized different earth-abundant metal catalysts, targeting the electrochemical reduction of CO_2.

He also synthesized metal complexes of tris(pyrazolyl) methane and tested them under electrochemical conditions, showing no activity towards the reduction of CO_2.

He attempted the synthesis of an organic macrocycle using acenaphthenequinone and dianiline (ether or amine) moieties.

A nickel-based catalyst featuring catechol and a diimine derivative of acenaphthenequinone as ligands has been identified and its synthesis has been attempted.

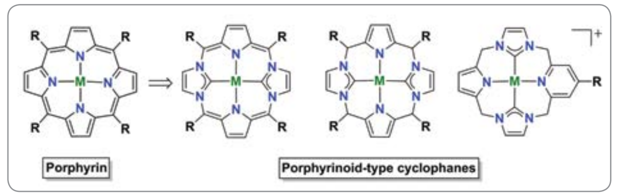
Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

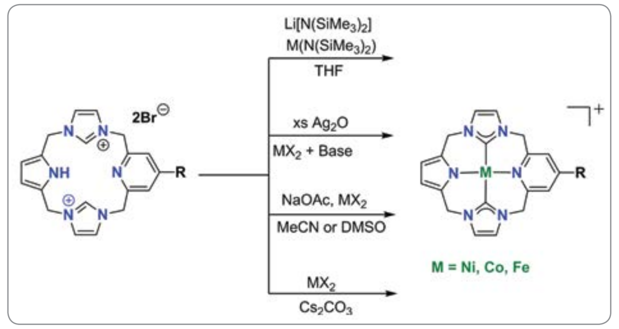
Samuel Sunday Hanson
Postdoctoral Fellow

THEME 3: CO_2 CONVERSION

Introduction

Porphyrin-based electrocatalysts for CO_2 reduction are amongst the best catalysts known to date. They feature an open site for CO_2 coordination and can be electronically modified. However, they are synthetically challenging to make and purify, and scale-up is almost impossible. Dr. Samuel Hanson, PhD, seeks to prepare porphyrinoid-type [NHC (N-heterocyclic carbenes)/pyridine cyclophanes) metal complexes which are relatively easy to make with huge scale-up possibilities, feature an open coordination site for CO_2 binding and boost of strong electron donation from the NHC motifs, and should lead to catalysts that can reduce CO_2 selectively, with high efficiency and at lower overpotential.





Results

Samuel has prepared some of the metal precursors in moderate to high yields and is currently carrying out metalation under various reaction conditions. Once prepared, these metal complexes will be characterized by single crystal X-ray diffraction (XRD), nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry (MS), and elemental analysis (EA), and their catalytic ability towards CO_2 reduction will be tested electrochemically using cyclic voltammetry and controlled potential electrolysis. The product(s) will be quantified using NMR spectroscopy and gas chromatography.

Conclusions

Samuel identified new ligand systems and metal complexes for CO_2 electroreduction.

He has achieved moderate to high yields for some of the ligands.

He is currently carrying out metalations under various conditions to find a suitable synthetic pathway to the metal complexes.

When the metal complexes are in hand, he will characterize those by single crystal XRD, NMR, MS, EA, and will test their catalytic ability electrochemically.

Samuel will disseminate the results of the research at various conferences and also will publish them in high impact journals.

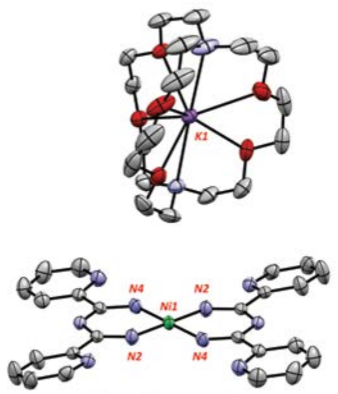
Can efficient, cost-effective CO_2 reduction catalysts be developed? (Synthetic fuels)

Novel homogeneous electrocatalysts for CO_2 reduction

Zachary Dubrawski
MSc student

Introduction

Recent literature infers design principles for molecular CO_2 reduction electrocatalysts. By applying these principles Zachary Dubrawski and his 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.



[K(crypt)][Ni(TAPPy)2]

Results

After some initial unsuccessful ligand platforms, Zachary has been focusing his attention on the 1,3,5-triazapentadienyl-2,4-bis(2-pyridyl) (TAPPy) platform. It has been shown that the Ni(II) TAPPy complex is catalytically active for CO_2 reduction to CO and carbonate ion (CO_3^{2-}) however, the compound decomposes before any meaningful catalysis can be realized. In the hopes of determining the mechanism for both reduction and decomposition, the chemical reduction of the complex gives [K(crypt)][Ni(TAPPy)$_2$] as an isolable solid which has been fully characterized (see figure). Zachary has found that the radical is of purely ligand character, characterized through electron paramagnetic resonance and high level calculations. Through reacting this compound with CO_2 he has determined that the complex operates through an outer-sphere electron transfer between the singly reduced species and CO_2 to generate the radical anion which then goes on to give CO and CO_3^{2-}. He is preparing a manuscript for publication on these results.

Conclusions

Zachary's findings suggest that Ni(TAPPy)$_2$ is a novel CO_2 reduction electrocatalyst that gives CO and CO_3^{2-} as C_1 products.

Chemical reduction of Ni(TAPPy)$_2$ gives [K(crypt)][Ni(TAPPy)$_2$] which has the radical located purely on the ligand framework.

Catalysis operates via an outer-sphere electron transfer to CO_2 to give the radical anion which then goes on to give the observed products.

CAN WE COST-EFFECTIVELY USE BIOENERGY FOR CO_2 CONVERSION? (BIOENERGY)

Marc Strous, Hector De la Hoz Siegler, Gregory Welch, George Shimizu, Jeffrey Van Humbeck, Joule Bergerson

THEME 3: CO_2 CONVERSION

Background

Bioenergy with capture and storage is a promising approach to realize the negative CO_2 emissions needed to keep global warming within safe limits. In this approach, biological carbon fixation converts CO_2 into biomass, which is converted to electricity in a power plant. The resulting concentrated CO_2 is buried via carbon capture and storage (CCS). Currently, high costs and high land use (competition with food production) lead to poor projected feasibility.

Research strategy

The Bioenergy research group is exploring innovations such as using high pH (more than 11) and alkalinity, using a natural microbial community instead of a specific algal monoculture, using biofilms instead of suspended cells, and conversion of the blue portion of the sunlight (not used by algae) into electricity using semitransparent organic solar cells. The group has also explored the use of metal organic frameworks (MOFs) for CO_2 capture. Techno-economic feasibility analyses have shown that for bioenergy applications the overall costs need to be reduced to $0.25 per kilogram of biomass. These analyses have also shown that photobioreactor construction and installation contribute to most of the costs and that effective light dilution will be crucial in realizing high CO_2 conversion rates per unit of land.

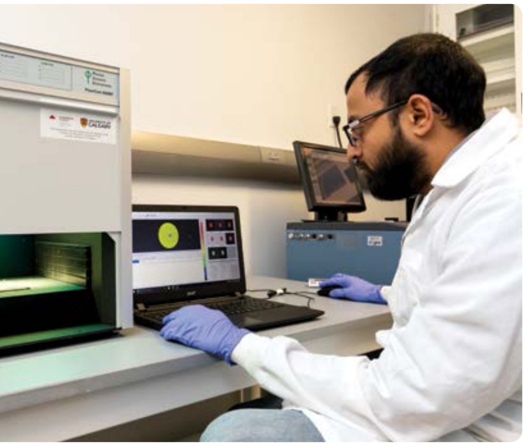
Desired outcomes

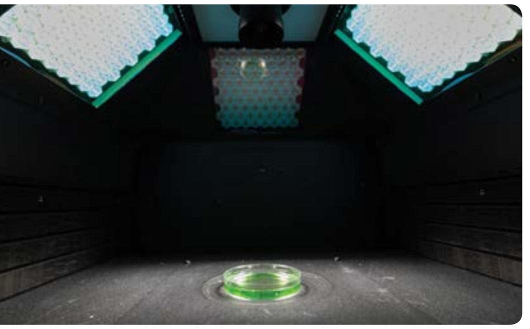
To address these points the research group has constructed a 10 square meters outdoor pilot plant (with SAIT), and have completed a photobioreactor manufacturing feasibility study (with third party experts). Progress on this project is also leading to (1) groundbreaking fundamental science for functional analysis of complex microbial communities; (2) unique capabilities for printing of large scale organic solar cells; (3) application of machine learning to enable discovery of new molecules for organic solar cells, with improved optical properties; (4) development of new options for downstream conversion of biomass into value-added products, to streamline commercialization; (5) development of new MOFs for air capture of CO_2.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Agasteswar Vadlamani

Postdoctoral Fellow





Introduction

Dr. Agasteswar Vadlamani, PhD, has started working on optimization of pH and alkalinity conditions to improve the productivity of phototrophic microbial communities. It is well established that high pH conditions will improve dissolution rates of CO_2 and that highly alkaline medium will provide sufficient inorganic carbon for microbial growth. However, identifying an initial pH range for a specific alkalinity medium is important. Identifying these parameters will not only result in improved efficiency of carbon capture from atmosphere but also provide sufficient inorganic carbon for phototrophic microbial growth.

Results

Though Agasteswar's main project is to optimize the productivity of phototrophic microbial communities, he initially focused on design aspects of an algal pilot plant for an outdoor solar technology facility. The design has successfully been validated and recently constructed at the University of Calgary. Thereafter, he shifted his research towards the cultivation aspects and productivity optimization of phototrophic microbial communities. He has identified the ideal pH range for growing microbial communities in medium alkalinity conditions similar to Soda Lakes. These parameters have been tested in laboratory environment. The cultivation conditions have significantly improved biomass productivities. Further, Agasteswar has been able to demonstrate that there are no detrimental effects of high carbonate concentrations on the photosynthetic parameters. Finally, he has shown the regeneration of spent medium by capturing CO_2 directly from air. Apart from optimization studies, he has also investigated the settling efficiencies of the mixed microbial communities. These results clearly indicate that concentrations of up to 10 per cent weight/weight (% w/w) solids can be achieved via settling.

Conclusions

- Designed an algal pilot plant for construction.
- Optimized pH and medium alkalinity.
- Significantly improved biomass productivities.
- Successfully demonstrated direct capture of CO_2 from air.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Alexandre Paquette

PhD student

Introduction

Microalgae are versatile, unicellular microorganisms that can be grown as immobilized biofilms with a high potential to capture CO_2, produce biofuels and bioproducts. To grow these microalgae, substantial amounts of nutrients such as nitrogen and phosphorus are needed. This large requirement of nutrients can be expensive and therefore nutrient recovery from the processed biomass is highly desirable for the sustainable growth of the microalgal biomass. With that in mind, Dr. Alexandre Paquette, PhD, aims to develop an economically-feasible and environmentally-friendly large-scale microalgae cultivation and conversion process in which all waste products are recycled back into the process as a nutrient source for algal growth.

Results

The total nitrogen initially in the media is depleted during algal cultivation. This means that the nitrogen will need be replenished for a new growth cycle. After one growth cycle there remains a sufficient amount of the other nutrients (potassium, phosphorus, sulfur, magnesium, calcium and iron) in the spent-media. This implies that the spent-media could be used again in another growth cycle, reducing the cost of replenishing the nutrients. Alexandre's research demonstrates the biomass elemental composition and enables rational design of a growth medium. This is an essential step towards implementing a nutrient recycling strategy. Finally, the above results illustrate the importance of understanding nutrient fate and microalgal composition to enable the effective reuse of spent-media for the regrowth of microalgae at high pH and alkalinity.

Conclusions

- There is a high potential for using the spent-media from algal cultivation for the regrowth of microalgae.
- Digested algal biomass can generate mineralized nutrients to be used for further cultivation.
- This information provides a path for developing a continuous system that could potentially enable complete recycling of nutrients from the biomass production and anaerobic digestion of the microalgae.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Audrey Laventure

Postdoctoral Fellow

Introduction

The overall goal of Dr. Audrey Laventure, PhD, and her research team, also featured, 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 (1) their lightness and flexibility, making them adaptable to the various form factors present in the photobioreactor and (2) their color-tunability, 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 a large area of red transparent OPV, acting both as light filters and collectors/convertors, leading to a self-powered photobioreactor.

Results

To achieve the project goal, Audrey and her team use a complimentary approach involving material design and preparation, small-scale performance optimization of the OPV and large-scale OPV coating. In the past year, the team has identified and optimized the upscaled synthesis of an organic red dye to filter the appropriate wavelength range. They have also optimized the performances of small-scale OPV (up to six per cent) by pairing their red dye with high performance semi-conductive polymers using green processing. The team has set-up four coating pieces of equipment for large-scale OPV production (two sheet-coaters and two roll-coaters) and have acquired slot-die coating expertise (easily transferable to roll-to-roll processing). They have coated large area organic films on flexible substrate to act as light filters. Currently, Audrey is optimizing the light filters to boost the algae growth and green-processing the ink formulation. She is also trying to achieve fully-printed and flexible large-scale OPV.

Conclusions

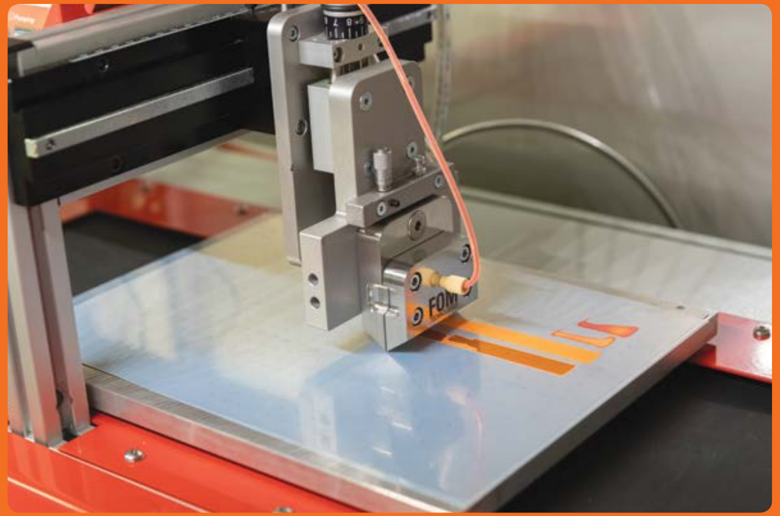
An organic red dye has been identified and its synthesis been upscaled.

OPV performances have been optimized for small-scale devices.

Slot-die coating has been used as a method to print large-scale flexible organic films to act as light filters to promote algal growth.

Audrey is currently transferring her skills to print large scale flexible OPV modules.

Dr. Audrey Laventure, PhD, acknowledges NSERC for a postdoctoral fellowship.



Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Cigdem Demirkaya
PhD student

Introduction

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 existing energy infrastructure. Cigdem Demirkaya's research project is the production of clean, low carbon and economically feasible biogas by anaerobic digestion of algae. The high pH and high alkaline growth conditions of algae, which increase CO_2 capture and algal productivity, bring some challenges to biogas production from algae. Challenges include ammonium inhibition and having reduced viability of methanogenic microbes. To achieve her goal, Cigdem adopted a two-phase anaerobic digestion process consisting of an acidification step followed by methanogenesis that will be applied to the system.

Results

Cigdem has performed the acidification experiments of algae by batch operation. The organic carbon content in the biomass is converted to volatile fatty acids by the autofermentation ability of algae. The volatile fatty acid production decreases the pH of the algae from 10.35 to 6.7, which is within an optimal pH range for methanogenic bacteria. The optimal pH and produced volatile fatty acids will help overcome the challenges that come from high pH and alkaline cultivation conditions. Results from the experiment have shown that there are many possible high value-added bioproducts that can be obtained from the different stages of anaerobic digestion while producing methane. These can be used to improve the cost efficiency of the process.

Conclusions

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 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.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

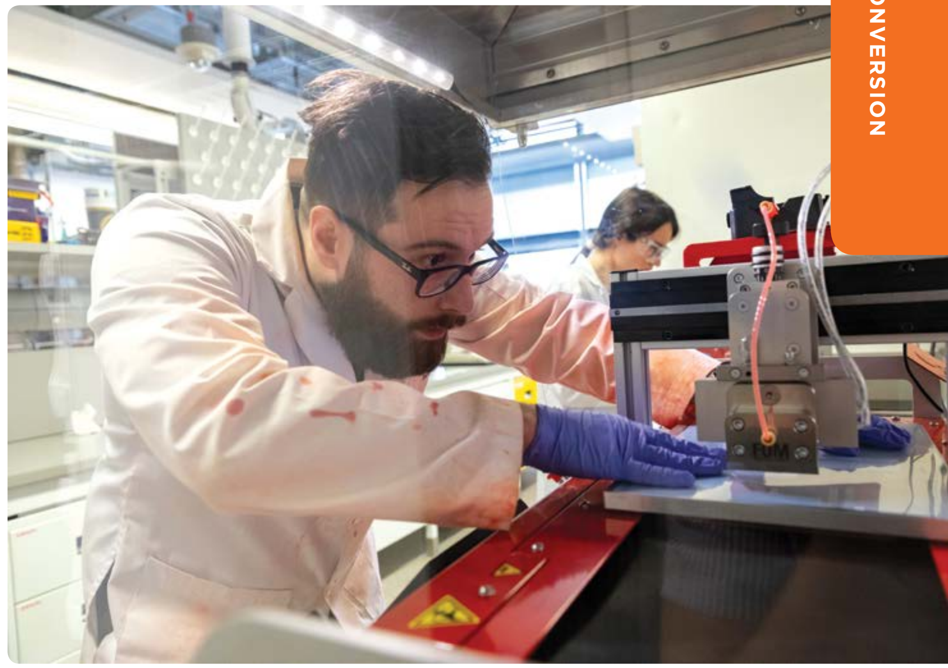
Edward Cieplechowicz
PhD student

Introduction

The overall goal of Edward Cieplechowicz's team, also featured, 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 (1) their lightness and flexibility, making them adaptable to the various form factors present in the photobioreactor and (2) their color-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

Edward's role within this project has been to develop new photoactive materials and establish large area printing conditions. He has demonstrated the efficient synthesis of champion photoactive materials on scales appropriate for photovoltaics (PV) module fabrication (more than 5 grams). He has developed a streamlined process for materials innovation to increase PV performance. Additionally, he has optimized printing conditions to deliver large area (10 by 30 cm) photoactive films on plastic substrates, fully laminated for use as optical filters. The next steps of Edward's research are to systematically vary material structures to further improve PV performance, establish a set of guidelines for evaluating the stability of the large area films and then learn the process for full PV module fabrication.



Conclusions

Edward has completed phase one of the project and has delivered flexible, red colored optical filters for use on the bioreactors.

He has established a streamlined procedure for materials innovation and the printing of large area photoactive flexible films.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

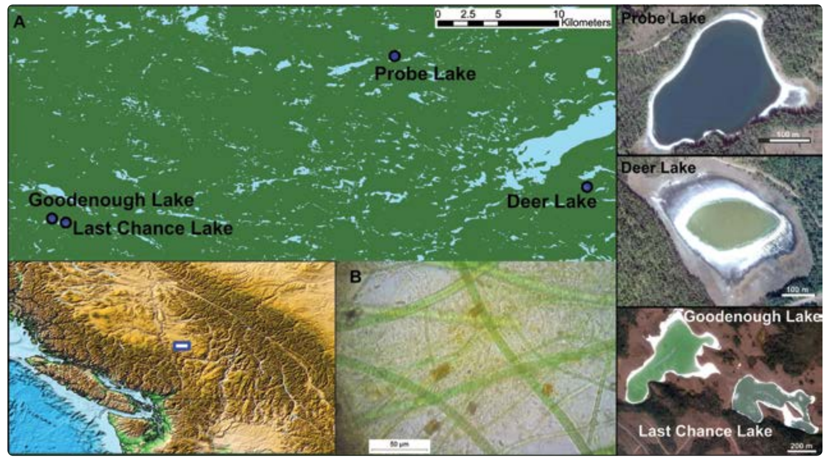
Jackie Zorz
PhD student

Introduction

Jackie Zorz works under the supervision of Prof. Marc Strous. She and her team are growing algae to capture carbon and for use as a starting material for downstream processing into commercial products like methane. For her project, Jackie is studying the ecology of the algae community, and the effect light intensity and quality has on growth and health of the algae system.

Results

The algae that grows in the lab bioreactors originate from the alkaline Soda Lakes in the interior of British Columbia. Jackie's first project has been to characterize the microbiology of these Soda Lakes using multiple "omics" techniques. Through this work, she has found that the Soda Lakes are very limited in nitrogen, contain many abundant species of cyanobacteria and that a quarter of the protein in the community is used for photosynthesis. Beyond the scientific value of this study, this information can be used in designing the lab bioreactors. Jackie's next project is to determine how the intensity and wavelengths of growth light affect productivity of the algae system at a detailed level. To do this, she will use fluorometry, mass spectrometry and gas chromatography analyses. The end goal of this project will be to incorporate organic solar cells, supplied by Prof. Gregory Welch's group, with the algae bioreactors to increase the overall efficiency of light harvesting.



Conclusions

The inoculum for the algae bioreactors come from the nitrogen-limited Soda Lakes that contain many diverse cyanobacteria species.

Preliminary results of Jackie's research suggest that the best light intensity for the efficiency of their algae system to be 150 micromole photons per square meter per second (μmol photons/m^2/s).

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Solid sorbents for CO_2 capture

Jian-Bin Lin
Research Associate

Introduction

This project has two main goals: (1) to advance a sorbent, CALF20, to a higher technology readiness level by exploring the stability and effectiveness of different structured forms needed to allow mass and heat transfer in a fixed bed and (2) to develop new structures based on a similar stable scaffolding for CO_2 removal from relevant gas streams including natural gas/shale gas upgrading.

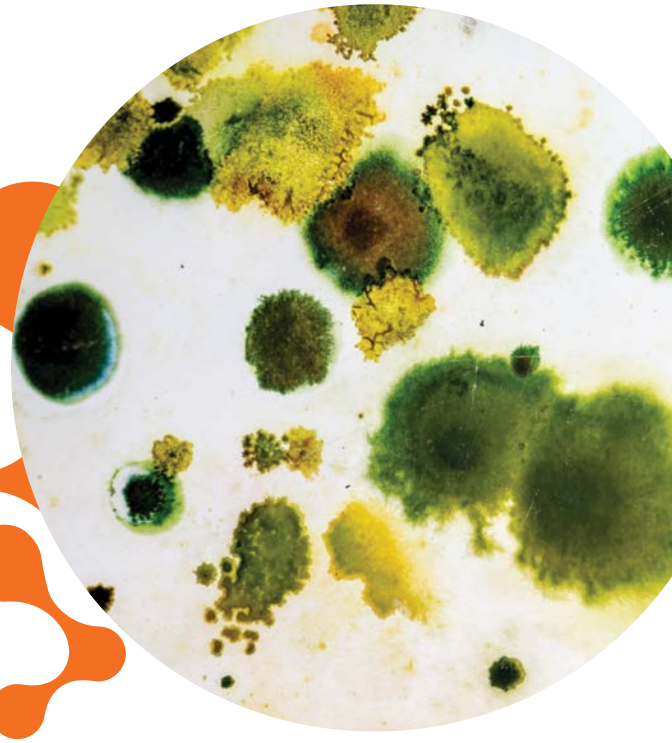
Results

Dr. Jian-Bin Lin, PhD, has been working partly as the departmental crystallographer for much of the past year. He has been successful in preparing several structured forms that are being tested with a collaborator for mixed gas and wet gas separations at the University of Alberta. A very good outcome is that the structured forms show good mechanical stability and the gas sorption properties of the metal-organic framework (MOF) are retained. A new MOF has been developed that shows the highest CO_2/CH_4 selectivity yet observed for an MOF.

Conclusions

A new promising MOF has been discovered with the highest selectivity for CO_2/CH_4.

Advances in structuring a patented MOF are ongoing and testing is promising. Notably, the lessons learnt from the first MOF will be transferred to the next.



Dr. Jian-Bin Lin, PhD, acknowledges Alberta Innovates Technology Futures (AITF) for funding and support.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

CO_2 conversion-CO_2 capture

Maria Camila Caceres Falla
MSc student

Introduction

In the effort towards net zero carbon energy, microalgal fuel promise to be one of the most complete solutions. Its production can be simplified in a three-step process involving carbon capture, algal biomass growth and conversion of biomass into fuels. CO_2 availability in the media is tightly linked with productivity of biomass and is limited by mass transfer and thermodynamic equilibrium, making it highly important to find a reliable, continuous and affordable carbon source for the growth of microalgae. The design of a carbon capture unit to deliver CO_2 to the microalgae is of high priority when working in a closed system. This unit is important because it takes CO_2 from the air and uses it to produce fuels, closing the carbon loop.

Results

For the first laboratory-scale absorption tower prototype, Maria Caceres Falla was only able to measure the change of the solution's pH with an external probe. Later, she constructed a second laboratory-scale absorption tower prototype with CO_2 composition sensors that have a 56 per cent efficiency of removing the CO_2 from the air and transferring it to the used media solution from the algae. These experiments have been conducted to develop and validate a model for the absorption to obtain the values for the pilot scale-up of the technology.

Conclusions

One theoretical plate is required to achieve a set removal of 75 per cent of CO_2 from air corresponding to a height of a theoretical plate of 1.2 meters. In her experimental results, Maria obtained a 56 per cent when the internal packings of the laboratory scale column have around 0.81 square centimeter (cm^2) packing area per cubic centimeter (cm^3) of column.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Self-assembling porous metal-phosphonate frameworks

Martin Glavinovic
PhD student

Introduction

Martin Glavinovic's project involves the design and synthesis of a stable microporous material that selectively adsorbs CO_2. His goal is to separate CO_2 from flue gas and then sequester it before emission into the atmosphere. The challenge is that flue gas has a low amount of CO_2 (5-15 per cent) and high humidity and acidity, which compete for and poison CO_2 binding sites. The proposed material is a hydrophobic molecular framework composed of metal ions and bulky phosphonate organic linkers. The building blocks are designed to self-assemble into a high surface area material held together by strong metal coordination bonds.

Results

So far, the major challenge has been the synthesis of the non-planar tris-phosphonate ligand, which is synthesized in seven steps. Martin has optimized the reaction conditions for each step and has synthesized the phosphonate ligand successfully at the 10-gram scale. The next challenge is to self-assemble the ligand with metals to yield an ordered porous framework. He designed the organic linker with a phosphonate functional group because they strongly bind to metal ions. Although this yields stable materials, metal phosphonates are frequently dense amorphous solids as they quickly precipitate out of solution. To address this challenge, the materials will initially be self-assembled with $[Cr(H_2O)_6]^{3+}$ to yield an intermediate hydrogen-bonded network that can be templated to give different structures. This can be dehydrated to yield a porous material with metal-phosphonate bonds. So far this strategy has yielded a crystalline hydrogen-bonded material, although the structure is yet to be confirmed.

Conclusions

Martin's project involves the synthesis of a hydrophobic microporous material that captures CO_2.

The material is composed of metal ions and organic linkers called ligands.

A novel phosphonate ligand has been synthesized in high yields.

Currently Martin and his team are self-assembling the material with $[Cr(H_2O)_6]^{3+}$ to yield ordered hydrogen- bonded materials.

Martin Glavinovic acknowledges NSERC CREATE and NOVA chemicals for their funding and support.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Marwa Abd-Ellah

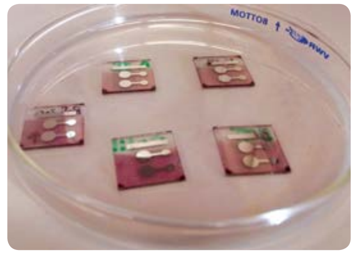
Postdoctoral Fellow

Introduction

The overall goal of Dr. Marwa Abd-Ellah, PhD, and her team, also featured, is to create a clean energy photobioreactor capable of reducing the CO_2 emissions and generating high value-added products. Organic photovoltaics (OPV) have been identified as a perfect matching technology because of 1) their lightness and flexibility, making them adaptable to the various form factors present in the photobioreactor and 2) their color-tuneability, enabling selective transmission of the appropriate photons that promote algae growth, and conversion of the non-transmitted light into electricity. Marwa's 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

To achieve the goal of the project, Marwa's team uses a complimentary approach involving material design and preparation, small-scale performance optimization of the OPV, and large-scale OPV coating. Marwa started on this project in fall 2018 and is currently investigating the cathodic interlayer using different wide bandgap semiconductor materials including ZnO, TiO_2 and SnO_2 as potential interlayers in their inverted structure for highly efficient lab-scale OPV systems. She has been optimizing the prepared interlayer either by doping, using inorganic or organic dopant, or by adding additional interlayers for better energy level alignment and device structure engineering. Fabrication of organic solar cell modules using slot-die printing methods, establishment of standard operating procedures and protocols for large area film formation and organic solar cell module fabrication are yet another sector Marwa has been working on. She has also been collaborating with the GRI research team by delivering flexible photovoltaic (PV) modules as prototypes in the integration of solar cells with bioreactors.



Conclusions

- Marwa is currently engaged in optimizing OPV performances for enhanced performance on the small-scale devices.
- She used slot-die coating as a method to print large-scale flexible organic films to act as light filters for promoting algal growth.
- She is currently transferring her skills to print large-scale flexible OPV modules.

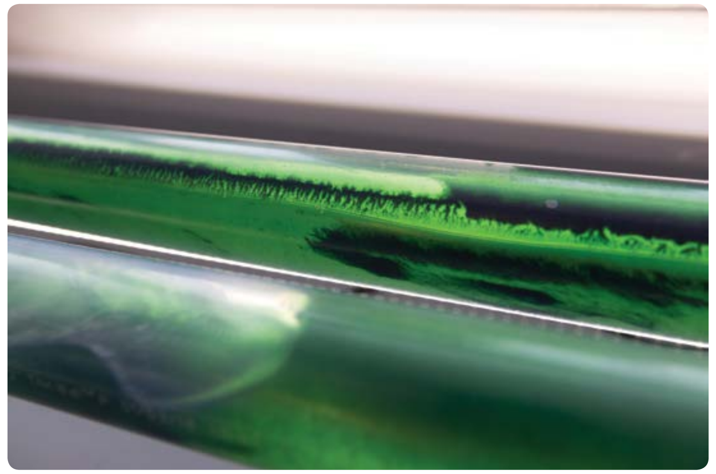
Dr. Marwa Abd-Ellah, PhD, acknowledges NSERC for her postdoctoral fellowship.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Ecophysiology of alkaliphilic cyanobacterial consortium

Maryam Ataeian

PhD student



Introduction

Maryam Ataeian works on biological carbon capture using microalgae. In this approach, microalgae converts CO_2 into biomass using light. The produced biomass can either be stored or serve as a carbon neutral source of energy. Current technologies are not suitable for large-scale operation due to high energy input demands and high costs. Maryam is optimizing the operation parameters of their system to obtain the highest productivity with maximum atmospheric CO_2 absorption. She is also characterizing the physiological response of the microbial community to different environmental factors, which enables her team to predict the community response in various conditions in large-scale operation.

Results

Maryam has been investigating the effect of high pH in combination with different sources of nitrogen on the productivity and growth of the existing microalgal test system. She has shown that by increasing the pH and providing sufficient carbon source, the atmospheric CO_2 uptake rate significantly improves. Her team, also featured, has also shown that their microbial community maintains its high productivity and photosynthetic activity even under harsh conditions. The productivity of the system is determined by the nitrogen source. Maryam analyzed the microbial community residing in the bioreactors and assessed the effect of changes in pH and nitrogen source on the community. She also evaluated the contribution of different populations in the community by studying protein expression.

Conclusions

- Increasing the pH maximizes the CO_2 absorption in the media.
- Type of nitrogen source is critical for productivity at high pH.
- Increase in productivity correlates with increase of microalgae in the community.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Maryam Nazari

PhD student

Introduction

Maryam Nazari's team has the overall goal of creating a clean energy photobioreactor capable of reducing the CO_2 emissions and generating high value-added products. Organic photovoltaics (OPV) have been identified as a perfect matching technology because of (1) their lightness and flexibility, making them adaptable to the various form factors present in the photobioreactor and (2) their color-tunability, 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

Maryam's role in this project is to fabricate photoactive devices with new materials and establish optimized conditions to achieve the highest efficiency. She has identified the best material in terms of efficiency and reproducibility and optimized the performances of small-scale OPV (up to 6 per cent) by pairing red dye to high performance semi-conductive polymers. The next steps in Maryam's research are to fabricate devices out of systematically variable materials structure to further improve photovoltaic (PV) performance, to establish the green-processing conditions and to achieve higher performance solar cells.

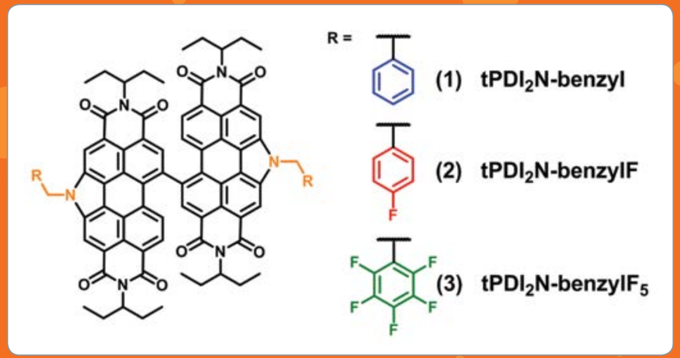
Conclusions

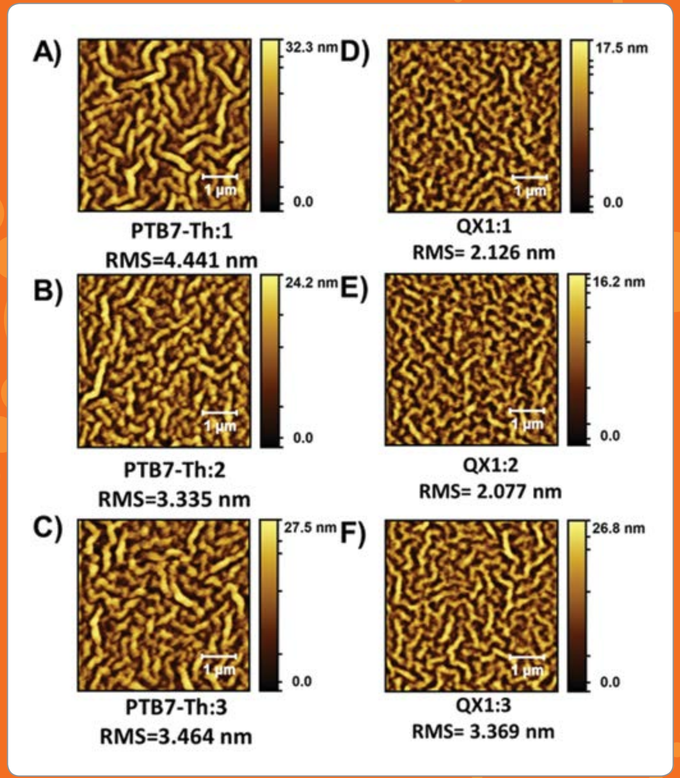
Maryam optimized OPV performances for small-scale devices.

She has tested new materials in the photoactive devices.

She is identifying and optimizing more efficient materials for the photoactive devices.

Maryam Nazari acknowledges the University of Calgary for the Eyes High post-graduate scholarship.





Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Creating a thin film of metal-organic frameworks on a substrate for enhanced mass flow

Nicholas David Fylstra
MSc student

Introduction

Removing CO_2 from fossil fuel emissions represents a solution to climate change during the transition to carbon neutral energy sources. However, the current costs to do this separation are very expensive. This project focuses on using solid sorbents, specifically metal-organic frameworks (MOFs), for post-combustion CO_2 capture in an effort to develop a more efficient and economical way to remove CO_2 from power plant emissions. MOFs resemble a fine crystalline powder after synthesis and the primary focus of this project is to add a mesoporous structure to the MOF to maximize mass transfer in this gas separation process.

Results

Nicholas Fylstra's research project is at the interface of materials chemistry and chemical engineering. Many early experiments imitating the literature focused on *in situ* MOF growth on a substrate has resulted in limited success. The original synthetic conditions of 180 C for 72 hours creates an environment that discourages heterogeneous nucleation on the substrate of the surface, resulting in some growth on the surface. Nicholas has shifted his focus to creating polymer composites using pre-synthesized MOFs and in creating different geometries from the traditional pellets used in a fixed-bed adsorption separation process. Particularly interesting is a composite MOF-polymer foam — MOF is used as the nucleating and blowing agent to create the foam — potentially giving a more direct control over the void spaces in a fixed bed. An overnight room temperature synthesis of the MOF has since been developed that suggests the *in situ* MOF growth experiments should be repeated.

Conclusions

- MOF structuring techniques must focus on scalability to be used in a process.
- Inducing heterogeneous crystal growth on a surface is difficult at high temperatures, though less intense synthetic conditions could resolve this.
- Maximizing the volumetric loading of the sorbent is a key component to a structure's mass transfer performance.

Can we cost-effectively use bioenergy for CO_2 conversion? (Bioenergy)

Taina Tervahauta
Postdoctoral Fellow

Introduction

The goal of this project is to convert solar energy into biofuel, CH_4, through microalgae cultivation and anaerobic digestion. Algae cultivation is done at high pH and alkalinity to improve CO_2 absorption and uptake. This, however, poses a challenge in downstream processing of algae where high pH can induce ammonia inhibition during digestion. By using autofermentation as a pretreatment step, the breaking down of algae biomass decreases the pH, avoiding ammonia inhibition during digestion. Additionally, high value-added products can be recovered in autofermentation, increasing revenue in the process. One of the main challenges is to implement successful recycling of CO_2, nutrients and trace elements to make biofuel production from algae economically feasible.

Results

Dr. Taina Tervahauta, PhD, aims for the successful breakdown of algae biomass during autofermentation decreasing the pH and enhancing methane production in anaerobic digestion. Her plan is to detect and extract high value-added products in autofermentation. She predicts that successful methane production from algae using short hydraulic retention time and long sludge retention time will allow low-cost digestion, resulting in high biomass conversion to CH_4. She is also aiming at a life cycle assessment (LCA) of the whole process, expressing technical and economic feasibility including carbon, nutrient and trace element mass balance, energy balance, and economic evaluation in comparison to other biofuel processes. Taina anticipates a few challenges with her research strategy. The substrate composition of the digester feed will change as a result of high value-added product recovery in autofermentation, for which the influence on carbon balance needs to be investigated. Extraction of high value-added products with high purity and low cost can be experimentally challenging. It is also challenging to stably operate high CH_4 yield digestion of algae with varying composition. Taina is also speculating the accumulation of toxins and inert material in nutrient and trace element recycling that can pose problems.

Conclusions

- Autofermentation as a pretreatment step prevents ammonia inhibition in anaerobic digestion of haloalkaline microalgae.
- High value-added product recovery in autofermentation increases revenue of algae conversion into biofuel.
- Short hydraulic retention time and long sludge retention time allow low-cost digestion with high biomass conversion into CH_4.
- Successful recycling of nutrients and CO_2 enable competitive biofuel production from algae.

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 Excellent 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 collaboration projects, involving more than 20 faculty members, with more than 30 graduate students and postdoctoral scholars. The universities have held three large joint workshops (fall 2017, spring 2018, fall 2018) for updating research progress collectively to the joint project participants.

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

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, Manisha Gupta

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

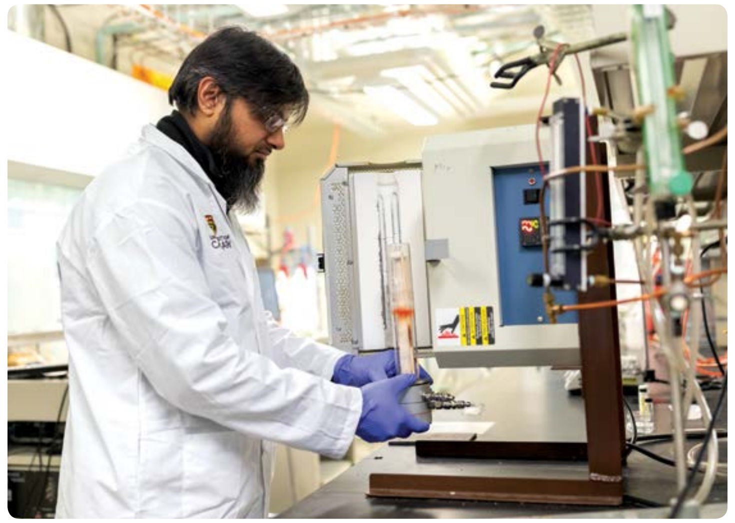
The primary outcome of this research will be a stable, high performing solid oxide electrolysis device that demonstrates tunable syngas production from CO_2 and steam at the cathode and emits a pure O_2 stream at the anode, while also serving to store renewable and excess grid electricity. A second major 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 Masood Ansari
Postdoctoral Fellow

Introduction

The project involves CO_2 conversion to useful chemicals using high temperature solid oxide electrolysis cells (SOECs). Dr. Haris Ansari, PhD, and his team have developed promising electrode materials that catalyze electrochemical CO_2 conversion efficiently with remarkable performance as either the fuel or air electrode. The team is developing a model experimental system, consisting of thin films of these electrode materials produced by pulsed laser deposition (PLD), in collaboration with Prof. Manisha Gupta's group at the University of Alberta. These thin films are amenable to fundamental studies to understand the intrinsic properties and underlying mechanisms behind the superior performance of the catalysts and tracking the stability of various interfaces during SOEC operation. This will help in the design and optimization of the catalysts to further enhance their performance in the future.



Results

Highly dense and crystalline pellets of $La_{0.3}M_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$ (M = strontium, calcium) (LMFCr) catalysts have been prepared and used as targets in the PLD system at the University of Alberta to deposit ca. 150–200 nanometer thin films on 10 millimeter by 10 millimeter (001)-oriented yttria-stabilized zirconia (YSZ) solid electrolyte substrates. Films of $La_{0.3}M_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$, grown at 700 C under 50–60 mTorr O_2 and 3 J/cm^2 laser fluence, have been found to be crystalline-as-deposited, single phase and epitactic on YSZ-(001), with a preferred orientation of (001). Although the aim is to obtain very smooth films with a surface roughness of approximately two to four nanometers, the surface roughness of Haris' films is currently approximately 50 nanometers. Efforts are underway to optimize the film growth parameters to reduce the surface roughness to the desired level before they can undergo in-operando electrochemical characterization under SOEC conditions.

Conclusions

$La_{0.3}M_{0.7}Fe_{0.7}Cr_{0.3}O_{3-\delta}$ thin films have successfully been grown on YSZ-(001) substrates by PLD.

The films grown at 700 C are crystalline-as-deposited, single phase and epitactic on YSZ-(001) with a (001) orientation.

Film growth parameters require optimization to decrease the surface roughness of the films for upcoming in-operando electrochemical characterization.

Dr. Haris Ansari, PhD, acknowledges the support provided by collaborators at University of Alberta.

Advanced electrochemical system for energy storage through CO_2 conversion

Oliver Calderon
PhD student

Introduction

Oliver Calderon's project uses X-rays produced by the synchrotron at the Canadian Light Source (CLS) to probe the mechanism of how CO_2 is reduced on the surface of perovskite materials — promising candidates for use in reversible solid oxide cells. Besides the obvious benefits of being able to remove CO_2 from the atmosphere, better understanding of this process will allow the researchers to more rationally design such devices in the future. This is vital since this technology is the potential backbone of a truly closed loop energy system and the environmental, economic and humanitarian benefits that entails.

Results

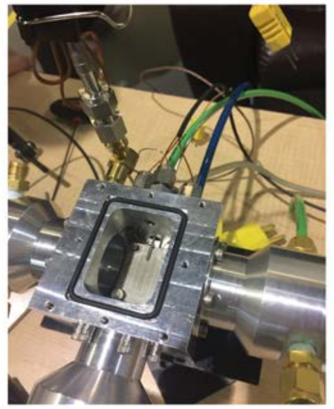
This challenging project brings together synthesis, design, engineering, device fabrication, electrochemistry and advanced characterization techniques. Oliver synthesized most of the target calcium and strontium containing perovskites. Early characterization indicates they have the desired composition and structure. Prototype button cells have been fabricated and successful electrochemical testing carried out. However, before large-scale optimization and testing could begin, the cell testing apparatus broke down. Oliver's team is now in the process of purchasing a unit and redesigning and repairing the current testers. Groundwork for the final operando testing rig has been laid in component procurement, 3D design and automation programming. Synchrotron beamtime has been applied for and obtained at CLS; unfortunately a major malfunction has suspended all activity at CLS. Luckily this setback caused Oliver to take a fresh look and resulted in new electrochemical CO_2 studies that complement the overall project but also represent potentially novel work.

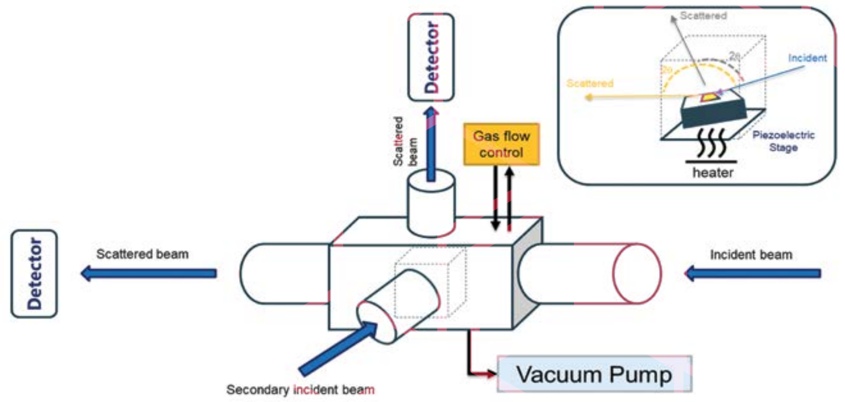
Conclusions

The potential impact of this project is immense and could lead to a truly closed loop energy system.

Progress made in synthesis, device fabrication, electrochemical testing, equipment procurement, automation programming and rig design is good despite apparatus malfunctions and facility shutdowns.

Setbacks have led Oliver to start exciting CO_2 studies that have not, to his knowledge, been undertaken before.





Custom *in situ* testing rig at the Canadian Light Source allows XAS analysis under single gas flow at high temperature.

Schematic of proposed *operando* testing rig. Fully modular system will allow XAS and secondary analysis under two gases or high vacuum, supplied independently to each electrode; under full electrochemical operation; and at high temperature.

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 near-field 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.

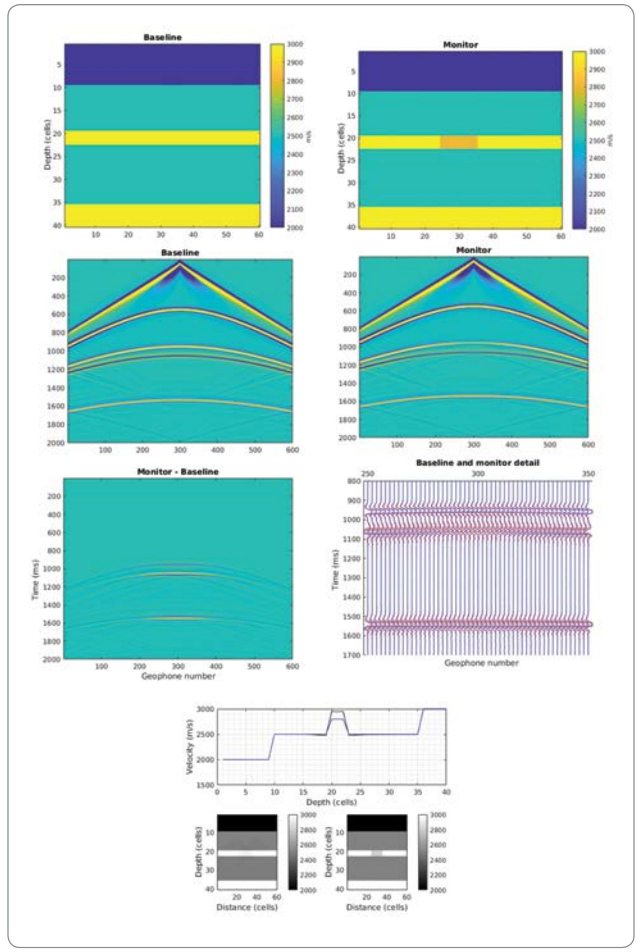
Thermal impacts for geological storage of CO_2

Jorge Enrique Monsegny Parra

PhD student

Introduction

Jorge Monsegny Parra is working on CO_2 capture monitoring by developing computer algorithms to elicit changes in subsurface elastic properties using seismic data. The challenges are to obtain a technique that is able to discern very small elastic changes that can cope with repeatability issues while also having a reasonable cost benefit. It is important to know the current state of the reservoir as CO_2 is being injected. Jorge aims to do this monitoring using seismic data to learn the changes in elastic properties that can be diagnostic of the reservoir state.



Results

Jorge has been successful in developing computer codes and programs that perform time-lapse elastic least-squares reverse time migration and full waveform inversion in CO_2 capture projects. He has also designed computer experiments with synthetic and real data showing the feasibility of the techniques, their expected results and how the programs should be applied. Some of the challenges that Jorge has faced in the project are that some small elastic changes could not be detected by the techniques, and imperfect seismic repeatability that can hinder the results. Also, the amount of computation could be a drastic limitation.

Conclusions

Being able to monitor the elastic properties of the reservoir in a CO_2 capture project is very important and time lapse versions of techniques like full waveform inversion and least-squares reverse time migration can accomplish this.

These time lapse techniques should cope with sensibility, repeatability and computational cost issues in a reasonable fashion.

Jorge Monsegny Parra acknowledges the support provided by CaMI-FRS Joint Industry Project subscribers.

Thermal impacts for geological storage of CO_2

Marie Macquet
Postdoctoral Fellow

Introduction

The goal of the Containment and Monitoring Institute (CaMI) Field Research Station is to develop and improve geophysical monitoring tools to detect potential leakage from a CO_2 storage site. For that purpose, different instruments are deployed and used on the field, including active seismic surveys (surface and downhole), straight and helical fiber optic cables, electrical resistivity tomographies (ERT), controlled source electromagnetic experiment and continuous seismic data. Dr. Marie Macquet's research will quantify the ability of these different methods (used separately or jointly) to detect the presence of CO_2 on the subsurface and determine their detection threshold.

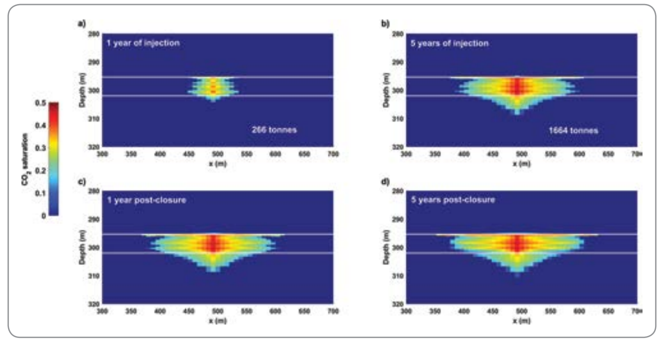


Figure 1

Results

Before any gas injection, surface seismic data is used to produce a feasibility study for CO_2 monitoring. It includes a reservoir simulation to determine the amount of CO_2 that can be injected in the subsurface injection zone, an analysis of the plume expansion behavior (Figure 1), and fluid substitution to estimate the changes in elastic parameters due to the injection. Marie has produced a synthetic seismic response to estimate the detectability of the CO_2 plume using surface seismic (Figure 2). She has used the results of fluid substitution to quantify the feasibility of the monitoring using other geophysical tools like distributed acoustic sensing and ERT. Additionally, Marie and her team are working with continuous seismic data at CaMI. Study of the micro-seismicity due to gas injection is the first way continuous data can be used. The second way is using interferometry to both image the subsurface and monitor the changes of velocities of the medium due to the presence of CO_2. This method is now widely applied at crustal scale and is starting to emerge at the exploration scale.

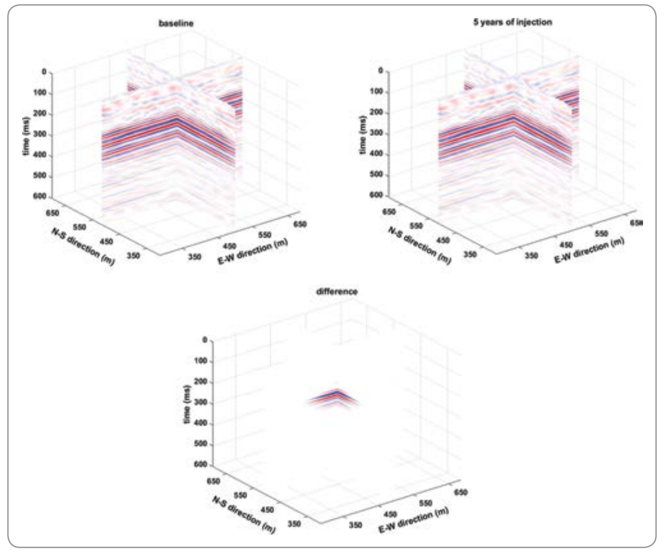


Figure 2

Conclusions

- Creation of a benchmark model used in different studies.
- Determination of detection threshold for potential CO_2 leakage using surface seismic.
- Application of emerging methods based on ambient noise correlation.

Dr. Marie Macquet, PhD, acknowledges the support of CaMI-FRS Joint Industry Project subscribers, Province of Alberta (Department of Environment and Parks) and the Government of Canada (Western Economic Diversification) for funding for the construction of the FRS; IHS Energy Canada for providing the wireline data; Cenovus Energy and Torxen Energy for kindly providing access to the CaMI field site; Schlumberger Carbon Services for providing Project Management during the development and construction of the Field Research Station.

Thermal impacts for geological storage of CO_2

Somayeh Goodarzi
Postdoctoral Fellow

Introduction

Dr. Somayeh Goodarzi, PhD, is researching thermal and geomechanical effects of injecting CO_2 into formations at different temperatures. It involves data analysis, coupled reservoir and geomechanical modelling, and computer programming. The injection data comes from the testing facility at the Containment and Monitoring Institute (CaMI) Field Research Station that was constructed by CMC Research Institutes and the University of Calgary to develop and calibrate monitoring technologies required for safe storage of CO_2. One of the most important aspects of this project is safety related to caprock integrity. The injection-induced poro-elastic and thermo-elastic changes can affect the integrity of the caprock and increase risk of leakage. The main achievement of Somayeh's research is a developed and calibrated coupled flow thermal and geomechanical model that can be used to mitigate the risk of leakage.

Results

The main outcomes of this research will be to identify the key variables that control caprock integrity and an improved understanding of the fluid flow and rock behavior under CO_2 injection at downhole pressure and temperature conditions. Somayeh's research will help develop a calibrated coupled flow thermal and geomechanical model that can be used to mitigate the risk of leakage. It will also help with increased quality of research based on planned collaboration with Canadian and international companies and universities. Working with real field data and having control of, and access to, an operation gives the research group and the University of Calgary a practical experience that was previously only available through oil and gas companies.

Conclusions

The main conclusion of the injection testing conducted so far are:

- Based on measured pressure difference between the two downhole gauges in the injection well, Somayeh and her team have identified that CO_2 phase changes are occurring in the well and this has thermal impacts.
- Thermally induced fracturing is possibly the cause of a rapid temperature drop in the injection well due to CO_2 gas expansion (Joule-Thomson effect).

Dr. Somayeh Goodarzi, PhD, acknowledges support from the University of Guelph G360, USDOE, UKCCSRC, SINTEF, NRCan, CMR, Shell, Chevron, Research Institute of Innovative Technology for the Earth, TOTAL, Equinor and Western Economic Diversification Canada.

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

Emilio Cavanzo Balcazar
PhD student

Introduction

Solvent-assisted steam recovery processes have the potential to produce heavy oil with less energy usage and greenhouse gas (GHG) emissions than thermal methods. A potential issue with these processes is that the condensing water can form a barrier to the mass transfer of solvent to the bitumen. Emilio Cavanzo Balcazar has developed a method to measure the diffusivity of hydrocarbon solvents in water. He also examines the role of gravity instability in enhancing the mass transfer rate.

Results

Emilio has designed an experiment to measure the mass transfer of a hydrocarbon solvent through a layer of water into a layer of bitumen below the water. The mass transfer rate is determined from the volume change over time of the bitumen layer which swells as the solvent enters the bitumen. Emilio is currently measuring mass transfer rates for three solvents at 20 C to 60 C and with different thicknesses of the water layer. A significant observation is that the bitumen layer swells upwards with a convex surface and not a flat surface. The surface curvature is likely because the bitumen phase becomes less dense than water when solvent enters the bitumen. The bitumen rises but is held back by surface forces at the wall. An important effect is that the bitumen is brought into close proximity to the solvent at the center of the surface, likely accelerating the mass transfer.

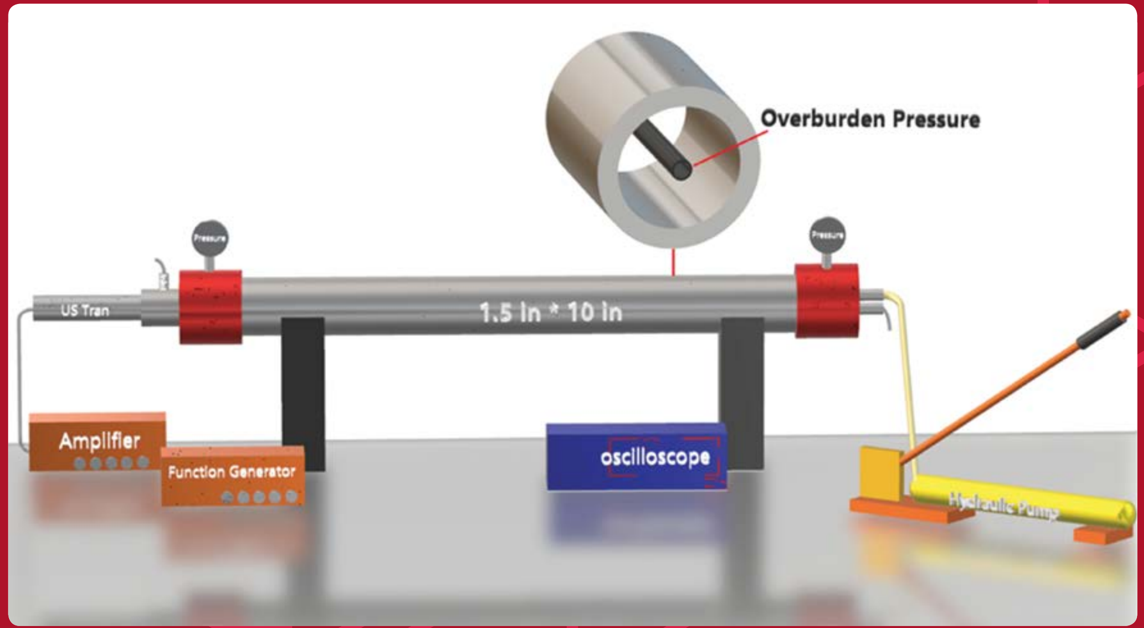
The next steps in this project are to:

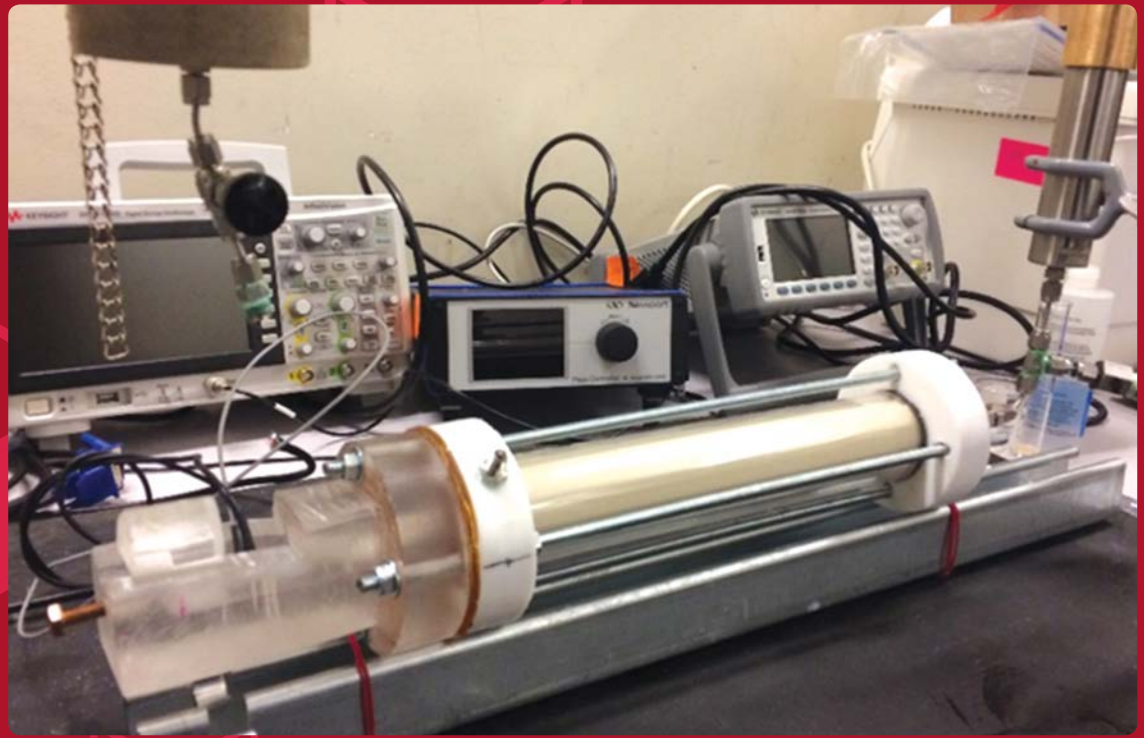
- Complete the mass transfer measurements.
- Develop a numerical mass transfer model to determine the diffusivity of the solvent through water as a function of temperature.
- Perform a qualitative analysis to assess under what conditions the curved interface becomes unstable.

Conclusions

During this research it was observed bitumen layer swells upwards with a convex surface and not a flat surface, likely because the bitumen phase becomes less dense than water when solvent enters bitumen.

Bitumen is brought into close proximity to the solvent at the center of the surface, likely accelerating the mass transfer.





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

Peyman Mohammadmoradi
Postdoctoral Fellow

Introduction

Dr. Peyman Mohammadmoradi's research addresses a few of the pressing questions that exist: (1) What are the correct physics regarding interfaces in bitumen-related recovery processes (e.g. steam/hot water with oil and water/solvent/oil production technologies)? (2) How can mass transfer be enhanced so that solvents become effective enough to replace water/steam? (3) Are there beneficial mechanisms in the recovery of bitumen through the excitation of interfaces using either acoustic or electromagnetic waves? (4) How can the pore level physics be modeled properly prior to scaling up for simulation?

Results

Peyman has built an experimental apparatus enabling direct vibration of pore fluids and visualization of miscible and immiscible fluids in 3D unconsolidated confined porous media. This helps to examine the effect of different parameters, including but not limited to, wave characteristics (shape, frequency, power, amplitude), pore fluid properties, solute type and concentration, injection rate and pressure, and overburden pressure, on the dispersion and mobilization in porous media. The sonic excitation of nanofluids in porous media has confirmed that the use of this technology can influence the solute transport by causing an increase in the pore velocity and dispersion. In conjunction with nano-assisted enhanced oil recovery (EOR) and stimulation technologies, this may lead to enhanced stability, dispersion, and transport of nanoparticles.

Conclusions

Peyman has built an apparatus and preliminary results have been obtained, with additional results expected in the near future.

Dr. Peyman Mohammadmoradi, PhD, acknowledges the University of Alberta in the joint program.

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

Destabilization of asphaltene stabilized water/model oil emulsions by ultrasound

Razie Khalesi Moghaddam
PhD student

Introduction

Water in oil emulsions is naturally formed because crude oil generally contains water. The water creates several problems and usually increases the unit cost of oil production. The currently available methods to separate water from oil are time-consuming and expensive. In this project, Razie Khalesi Moghaddam is examining a new way to destabilize these emulsions using ultrasounds. This method has the potential to be faster and more energy efficient than current technologies and does not require chemicals. Ultrasound radiation can desorb asphaltene (emulsion stabilizer) from the interface and increase the chance for coalescence of water droplet by perturbing oil-water interfaces.

Results

Razie has evaluated the effect of ultrasound radiation on the bulk of emulsions as a proof of concept and she has observed that the size of water droplets increases with ultrasound treatment (increase of coalescence). Also, she has analyzed the team's model system in terms of asphaltene concentration and solvent composition by interfacial elasticity measurements as the most stable case to coalesce. Razie, along with her team, is currently designing an experimental apparatus to develop controlled ultrasounds and enable visualization of the interfaces *in situ*. This apparatus will be coupled with optical tweezers to measure local forces between droplets.

Conclusions

Droplet size of water in model oil is increased in the presence of ultrasound radiation. This demonstrates that ultrasound radiation can destabilize water in oil emulsions.

Microstructural investigations of water in oil-asphaltene stabilized interfaces in the presence of ultrasounds are currently being performed.

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

Benjamin O. Edafiaga

MSc student

Introduction

The intent of Benjamin Edafiaga's project is to design optimized steam-based recovery processes for oil sands reservoirs. The net present value (NPV) will be optimized for a steam-assisted gravity drainage (SAGD) operation by altering the operating strategy of the steam-based recovery process and the well configuration. In the traditional SAGD method, the main drive for bitumen production is via gravity drainage. To increase the rate implies that additional forces have to be used — the well configuration will be altered to determine if pressure drive can augment the production rate and recovery. Different optimization techniques will be explored; this includes stochastic methods and hybrid methods.

Results

So far, Benjamin has performed a detailed literature review of optimization studies of SAGD and thermal-solvent recovery processes and explored a hybrid optimization technique using both simulated annealing and a genetic algorithm.

Conclusions

The literature review revealed that nearly all optimization studies focus on using the SAGD well architecture and that alterations to the well configuration has not been done by using optimization methods.

Results so far demonstrate that hybrid optimization algorithms can take advantage of the benefits of the individual methods yielding faster optimization runs.

The generated NPV results could be used for forecasting production investments, trends and returns profiles for better planning, cost savings and revenue generation outlooks and profiles.

Benjamin Edafiaga acknowledges Computer Modelling Group for use of STARS™ and Schlumberger for use of Petrel and Eclipse.

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

Mahta Vishkai
Postdoctoral Fellow

Introduction

Dr. Mahta Vishkai, PhD, explores the optimization of steam-assisted gravity drainage (SAGD) in a detailed point bar geological model. The key cost and generator of greenhouse gases in SAGD is steam generation. Also, large amounts of water are consumed in the process. The goal of this project is to achieve a minimum steam-to-oil ratio since the steam represents operating cost and produced oil represents process revenues. Mahta has constructed an ultra-refined point bar model based on geological and seismic information. The operation of the SAGD well pairs will be optimized for the pad-scale model by using an evolutionary optimizer.

Results

At this point, the model has been constructed and is ready to run. Due to the heterogeneity of the point bar, the steam chambers that form in the reservoir are heterogeneous; in other words, steam chamber conformance is poor. The point bar pad-scale model takes a long time to execute and methods to accelerate its run time are being explored. One method being explored is to perform a very coarse grid and low solver tolerances for the first set of runs and as the optimization method starts to converge, to then tighten the tolerances on the solver.

Conclusions

A detailed point bar model has been constructed and is ready for SAGD optimization.

Run times for the model are large and methods to accelerate the optimization runs are being explored.

The changes of the operating strategy that will be done to optimize the performance of SAGD will be constrained to about 10 per cent changes from current average operations in the field. This imposes that the strategy is not too radically different from current operations but also explores how relatively small changes to the operation can yield large cumulative effects on the performance of the recovery process.

Dr. Mahta Vishkai, PhD, acknowledges Computer Modelling Group for use of STARS™ and Schlumberger for use of Petrel and Eclipse.

LIFE CYCLE ASSESSMENT OF ENERGY SYSTEM TRANSITIONS

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

UCalgary Team: **Joule Bergerson**

UAlberta Team: Amit Kumar, Theme Leads for Solar, Theme Leads for Wind, Theme Leads for Biomass, Theme Leads for System-Wide

Background

There has been a shift in life cycle assessment (LCA) modelling techniques over the past decade from attributional to consequential. Consequential techniques have attempted to address the fact that the standard attributional LCA (one direct energy supply chain at a time) typically generates results in terms of a unit of output and misses the dynamic shifts throughout the economy that could occur if a new technology pathway gains market share. In addition, the full magnitude of the impact that is possible by deploying a new technology in the economy is generally absent or imprecisely characterized using attributional methods. Consequential techniques rely on macro-economic models; however, these models are not technology-rich, do not normally have the capacity or mandate to explore the role of technology innovation in transitions, and, to date, have primarily focused only on some biofuel pathways. This could lead to potential unintended environmental consequences as well as missed economic opportunities.

Research strategy

The focus of the present project is to close the knowledge gap and understand the environmental impacts economy-wide and globally of different energy transition pathways.

Desired outcomes

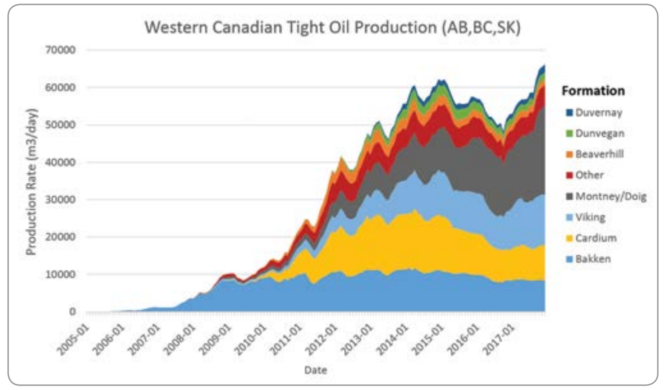
As a result of these studies, techniques will be developed and results will be obtained that will provide insights which can help guide/inform policy and technology development. The results and insights will help Albertan and Canadian policy makers understand the full consequences of different pathways at a global scale. This will better equip them to make decisions about investments and policy development and position Canada for further discussions on mitigation of greenhouse gas (GHG) emissions at a global scale. This will help Canada in negotiating the global GHG mitigation agreements with other countries and the United Nations similar to the Paris agreement. This will also help in inter-provincial negotiations under the Pan-Canadian framework. The information developed in this proposed project will aid in the development of a robust Pan-Canadian and global energy strategy.

Life cycle assessment of energy system transitions

Alexander Bradley
MSc student

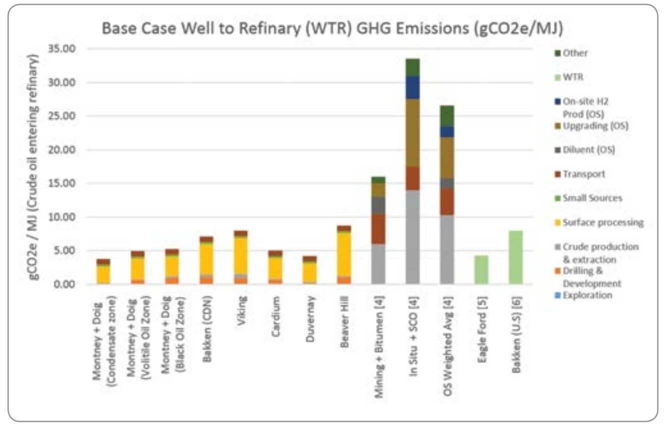
Introduction

The objective of Alexander Bradley's research is to conduct a life cycle assessment (LCA) on the production and use of Canadian tight oil resources. Tight oil requires the combination of hydraulic fracturing and horizontal drilling to be produced economically. Canada is home to significant tight oil resources and production is expected to grow over the coming decades. This study will determine the greenhouse gas (GHG) emissions and freshwater use associated with producing tight oil from different Canadian formations. Furthermore, a consequential LCA will be conducted to determine the social, economic and broader environmental impacts of the Canadian tight oil industry. The results of this research will demonstrate the environmental trade-offs between tight oil development decisions and the consequential impacts of current and future production.



Results

Alexander's research to date has collected and assessed a vast amount of upstream data relating to oil and gas production within Canada. The availability of data and the method used for reporting differs significantly between each province. Understanding these differences and where gaps in data exist has been an important process in the early stages of his research. A model has been developed to determine the upstream (drilling, producing, processing and transporting) GHG emissions resulting from tight oil. Base case scenarios show emissions from Canadian tight oil are lower than oil sands and conventional US production. Future work will focus on assessing uncertainty, modelling refinery and downstream emissions, and understanding the consequential impacts of production. The results of the study will be compared to a renewable energy system pathway evaluated by University of Alberta researchers.



Conclusions

- Base case GHG emissions from Canadian tight oil are lower than oil sands production.
- GHG emission intensities vary between producing formations.
- Flaring and venting is a key driver in upstream emissions.
- Water use for hydraulic fracture treatments varies largely for different Canadian tight oil formations.
- Environmental trade-offs should be considered in development decisions.

Alexander Bradley acknowledges collaborators at the University of Alberta.

COMPUTATIONAL SEISMIC FULL WAVEFORM INVERSION

UCalgary Team: **Kristopher Innanen** • UAlberta Team: Mauricio Sacchi

Background

One of the primary challenges facing 3D exploration and monitoring seismic technology in the coming five to ten years is to formulate, validate and bring online the set of procedures known as seismic full-waveform inversion (FWI) as applied in onshore reservoir (particularly unconventional) environments. FWI has met with considerable success in marine applications as a technique for creating high-resolution velocity models, a key input for seismic image formation. However, the issues arising when geological properties other than P-wave velocities influence seismic waveforms have not yet been completely addressed.

Research strategy

In onshore reservoir settings, where variations in many elastic and/ or rock-physics properties must be simultaneously determined, these "multi- parameter" issues come directly to the forefront. The goal of this project is to incorporate multi-parameter elastic FWI with anisotropic variants (for fracture characterization) and viscoelastic variants (for viscosity characterization) into the unconventional reservoir surveillance world. In addition to managing computational boundaries so that domains are manageably small, the massive data sets associated with full 3D seismic must be incorporated into the simulation carefully. Encoded supergathers of data permit large swaths of data to be injected into FWI propagation/simulation stages simultaneously as opposed to serially (as standard theory requires). This, in principle, reduces the computational burden many-fold.

Desired outcomes

As an outcome of this project, 3D finite difference forward modelling of elastic anisotropic seismic wave codes with new hybrid boundary conditions designed to reduce boundary effects will be developed and implemented. This reduces the size of the computational volume and therefore the computational burden of FWI. Also, design, via adjoint state techniques, of algorithms to compute FWI gradients for horizontal transverse isotropic (HTI) or tilted transverse isotropic (TTI) media can be anticipated. This supports the growing FWI numerical toolbox and will enable the important problem of parameter-resolution analysis. Multiparameter elastic/anisotropic FWI for fracture surveillance with techniques of blended acquisition/processing will be merged. This reduces the number of seismic shot records input into the gradient calculation.

Computational seismic full waveform inversion

Junxiao Li
Postdoctoral Fellow

Introduction

Dr. Junxiao Li, PhD, focuses on developing and publishing new computational schemes (pseudospectral, finite difference) designed to simulate seismic waves and to compute full-waveform inversion (FWI) gradients with application to 3D anisotropic inversion. Junxiao also works with other postdoctoral scholars on merging new computational FWI schemes with state of the art multicomponent land seismic data and on validating multicomponent elastic FWI on physical modelling laboratory data acquired at the University of Calgary.

Results

Junxiao has achieved pseudospectral time-domain forward modelling to model separate seismic wave modes (qP-, qSV- and qSH-wave) in vertical transverse isotropic (VTI) media in which the hybrid-perfectly matched layer (H-PML) method, that eliminates artificial boundary reflections, is also transferred into the wavenumber domain. The qSH-wave simulation is based on reducing the second order wave equations into first order system and the staggered-grid finite difference method is then applied into the wavenumber domain. For the qP- and qSV-wave simulation, the above method is proven to be not applicable to do the forward wavefield simulation, instead, a new approximation of the decoupled qP- and qSV-wave equation set is proposed and simulated using pseudo-spectral time-domain forward modelling, in which the H-PML is applied into the second order wavenumber domain wave equations. Additionally, for the frequency domain FWI in VTI, Junxiao applied the frequency-selection strategy moving from lower to higher frequencies. The elastic constant parameters C_{44} is first inverted, then C_{11}, C_{33} are inverted after the C_{44} is first inverted. The inversion results for these three parameters are to be used during the inversion of C_{13}.

Conclusions

Junxiao proposed a temporal fourth-order scheme for solving the elastic shear (SH) wave equations in VTI media, which appears to suppress wrap-around and Gibbs' artifacts, noted in other methodologies when waves propagate through heterogeneous formations.

He has proposed a new approximation of the decoupled qP- and qSV-wave equation set and simulated it using pseudo-spectral time-domain forward modelling. The H-PML is applied into the second order wavenumber domain wave equations.

The frequency-selection strategy used in the frequency domain FWI is able to invert the elastic constants effectively.

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 transitions

Susanna Afra Maria Rijkhoff
Postdoctoral Fellow

Introduction

Dr. Susanna Rijkhoff, PhD, seeks to understand under what circumstances citizens are supporting environmental policies and willing to participate and cooperate in the implantation of these policies. She focuses on several aspects: beliefs and perceptions about climate change, the communication (message and messenger) of policy initiatives and obstacles for citizens to collaborate. These obstacles can be attitudinal (e.g. distrust, cynicism) or more tangible (e.g. time, money). It is desirable to create mutual understanding and collaboration by finding the most appropriate ways of communication, about climate change and necessary policies and action, between the government, the oil and gas industry, civil society and individuals.

Results

Currently the project is in the design phase to start the first large data collection in 2019. This includes a large online survey and experiments. For the design of the study, Susanna has searched for existing literature pertaining to this topic to seek information about current unanswered research questions and the particular question wording for the survey part of the data collection. As an expert in public opinion and political behavior, Susanna contributes measurements of attitudes that are important in citizens' support and potential cooperation for environmental policies (e.g. cynicism, distrust and efficacy). In addition, her skills in political communication will inform the project's approach to reach citizens in an effective manner.

Conclusions

There are no specific outcomes yet as data still needs to be collected.

Susanna has designed a solid survey with appropriate questions and question wordings. Her efforts will also lead to a good experimental design that will be included in the survey to understand citizens' reactions to particular messages and messengers.

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.

ENGINEERING AND DEVELOPING ADVANCED CATHODES FOR PROTON CONDUCTING SOLID OXIDE FUEL CELLS USING ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY GENETIC PROGRAMMING

UCalgary Team: **Venkataraman Thangadurai,** Viola Birss

Technion Team: Yoed Tsur, Maytal Caspary Toroker

Background

Proton conducting solid oxide fuel cells (H-SOFCs) are promising energy conversion devices because they can operate at low temperature range (400-700 C) and increase the market acceptability. However, their practical application is limited due to lack of high performance electrode (cathode) material at low temperatures. While the research on developing novel mixed ionic and electronic conducting (MIEC) cathodes is underway, the understanding of the fundamental electrochemical processes for electrode reaction is still lacking. Gaining this understanding can guide researchers towards engineering new materials.

Research strategy

The aim of the present project is to develop novel cathodes, SOFCs and solid oxide electrolysis cells (SOECs) along with exploring the fundamental electrochemical processes for oxygen reduction reaction (ORR) that control the performance of SOFCs and SOECs.

Desired outcomes

Firstly, the key goal is to develop novel metal oxide electrodes for SOFCs and SOECs. Secondly, establishing the electrochemical impedance model for SOFC/SOEC operation based on evolutionary electrochemical impedance spectroscopy genetic programming (ISGP) and density functional theory (DFT) analysis. Additional a link will be established between ORR properties of MIEC perovskites to fuel cell performance. Lastly, the project will provide an understanding of the electrochemical performance of mixed ion and electron conducting perovskites as a function of temperature and oxygen partial pressure using ISGP and DFT.

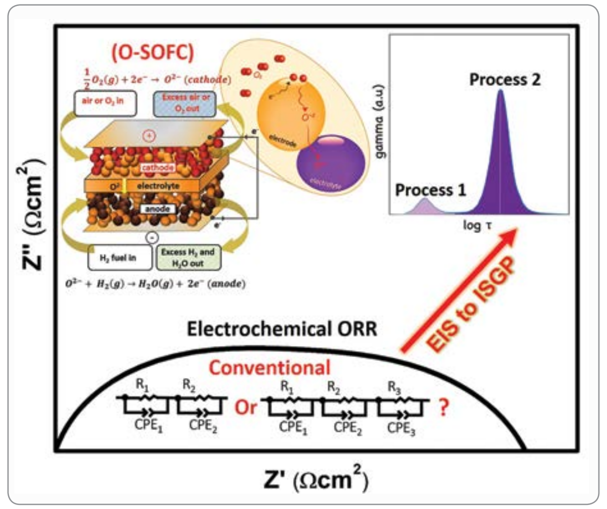
Engineering and developing advanced cathodes for proton conducting solid oxide fuel cells using electrochemical impedance spectroscopy genetic programming

Kalpana Singh

Postdoctoral Fellow

Introduction

As the practical application of proton conducting solid oxide fuel cells (H-SOFCs) is limited due to lack of high performance cathode material, Dr. Kalpana Singh, PhD, and her research team have developed cobalt-free cathodes. However, as it is very difficult to elucidate oxygen reduction reaction (ORR) steps with similar relaxation times using conventional equivalent circuit modelling, electrochemical performance for ORR has been investigated through impedance spectroscopy genetic programming (ISGP). Through ISGP approach, it has been possible to gain additional information, which may be convoluted and therefore undetected in conventional alternating current impedance analysis.



Results

Kalpana's past research has shown the effect of copper (Cu) substitution on the oxygen non-stoichiometry, chemical capacitance and ORR properties of $Ba_{0.5}Sr_{0.5}Fe_{1-x}Cu_xO_{3-\delta}$ (x = 0-0.20, BSFCu). Electrochemical performance for ORR has been investigated through ISGP. Contrary to common understanding, ORR properties of BSFCu +$La_{0.8}Sr_{0.2}Ga_{0.8}Mg_{0.2}O_{3-\delta}$ (LSGM) electrodes decreases with the increase in Cu-content. Chemical capacitance values decrease with increase in Cu content at all temperatures. Thermogravimetric analysis has shown that with the increase in Cu content, the weight loss and hence oxygen loss also decrease. These results indicate that the best performance seen with lowest Cu content is due to its inherent ability for high non-stoichiometry at operating conditions. The lowest area specific resistance value [0.135 ohm square centimeter (Ω cm^2)] and hence best electrochemical performance is obtained for BSFCu005+LSGM at 700 C under air. These results suggest that there is an optimal doping amount of Cu after which ORR properties decrease in BSFCu compositions.

Conclusions

Kalpana made a successful visit to Technion in Israel where she performed additional experiments including dilatometer, scanning tunneling electron microscopy and X-ray photoelectron spectroscopy and learned impedance spectroscopy genetic programing techniques.

She has explored $Ba_{0.5}Sr_{0.5}Fe_{1-x}Cu_xO_{3-\delta}$ (BSFCu) cathodes.

An optimal Cu-doping amount for better electrochemical properties is 0.05 for BSFCu compositions.

Dr. Kalpana Singh, PhD, acknowledges the support of her collaborators at Technion — Israel Institute of Technology.

CONVERSION OF CO_2 TO SYNGAS USING PEROVSKITE-BASED SOLID OXIDE ELECTROLYSIS CELLS

UCalgary Team: **Simon Trudel,** Viola Birss, Sathish Ponnurangam

Technion Team: Maytal Caspary Toroker

Background

Conversion of CO_2 using solid oxide electrolysis cells is achieved by using energy from environmentally friendly sources and a mixture of water and/or CO_2 on an electrocatalyst at high temperatures. The use of perovskites from earth-abundant materials as electrocatalyst is of great interest because they have shown improved efficiencies compared to other materials like alkaline cells. On a fundamental view, an atomistic knowledge of the mechanisms involved in CO_2 conversion on perovskites is far from complete. A full understanding of such mechanisms is necessary to comprehend the effects of temperature, the electric field applied and the perovskite composition that will allow optimization of the conversion.

Research strategy

For this project, a reactive molecular dynamics method, ReaxFF, will be used to model the chemical changes leading to syngas formation involving two perovskites, $La_{0.3}Sr_{0.7}Fe_{0.7}Cr_{0.3}O_{6-\delta}$ and $La_{0.3}Ca_{0.7}Fe_{0.7}Cr_{0.3}O_{6-\delta}$, and mixtures of CO_2, CO, and water. ReaxFF makes use of quantum mechanical data to model the interactions between the different atoms including formation and breaking of bonds. However, because of the diverse conditions involved in this study (i.e. temperature, electric field, material compositions, etc.) refinement of the parameters used by ReaxFF is necessary. To this end, density functional theory (DFT)-based calculations of the materials will be used to generate a dataset to train the force field and improve its accuracy.

Desired outcome

The desired outcome of this project is to elucidate the mechanisms involved in the CO_2 electroreduction using perovskite-based electrolysis cells. Results from this project will allow researchers to pinpoint the elementary steps of reaction and the effect that temperature, electric field and composition of the perovskite have on them. With this understanding, maximal efficiency of the CO_2 conversion using electrolysis cells can be achieved.

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

Franz Michel Martinez Rios
Postdoctoral Fellow

Introduction

The goal of Dr. Franz Martinez's project is to convert CO_2 and water to syngas using a perovskite electrocatalyst that is made of earth-abundant materials. The specific objective of his project is to optimize the composition and structure of the perovskite catalysts using a computational approach. This encompasses the modelling of processes occurring between CO_2 and the interface of electrode-based-perovskites used in solid oxide electrolysis cells. One of the outcomes of this project is to understand the variables that drive the electroreduction of CO_2, which in turn will allow a better control of its conversion in electrolysis cells.

Results

The main results that Franz has obtained so far are regarding the development of a density functional theory (DFT)-based reactive force field for modelling the system. The developed force field, in prototype form, shows that under standard temperature and pressure conditions, the CO_2 tends to get adsorbed on the surface of the $La_{0.7}Ca_{0.3}Fe_{0.7}Cr_{0.3}O_{6-\delta}$ perovskite. Chemisorption is observed between one of the oxygen atoms of the CO_2 and chromium (Cr). It also leads to the formation of carbonate on the surface in some cases. More improvements of the force field are necessary as it is in the very early stage of development, nevertheless, the results are promising as both trends can be observed from DFT methods.

Conclusions

Prototype reactive force field is capable of reproducible results from DFT methods.

Full development of the reactive force field will allow for modelling of the processes and reactions occurring between the perovskite and CO_2 at higher temperatures.

Dr. Franz Martinez, PhD, acknowledges the computing resources provided by Compute Canada.

NEXT GENERATION FUEL CELL AND CO_2 SEPARATORS BASED ON ANION EXCHANGE IONOMERS

UCalgary Team: **Kunal Karan,** Sathish Ponnurangam

Technion Team: Dario Dekel, Viacheslav (Slava) Freger, Tamar Segal-Peretz

Background

Anion exchange (AE) ionomers can be thought of as polymers containing anions or simply polymers to which alkali groups are tethered. They have garnered tremendous interest for electrochemical energy conversion and storage (ECS) devices because (1) they maintain alkaline pH allowing the use of inexpensive metal catalysts, and (2) can be synthesized from low cost hydrocarbon polymers. The research group is focusing on two such ECS devices — hydrogen fuel cells and CO_2 electrochemical reactor. The electrodes of AEM (anion exchange membrane) fuel cells (AEM FCs) and AEM-based electrochemical CO_2 reactors are a nanoporous nanocomposite of electrocatalysts covered by ultra-thin (a few nanometers) ionomer films. The ionomer-catalyst interactions control the interfacial electrochemical kinetics and the structure/properties of ionomer thin films control the long-range ionic transport. Thus, the ionomer thin films control the transport and kinetics in the electrodes of the aforementioned electrochemical devices. There are practically no studies reported on the structure and properties of AE ionomers at the nanometers-thin scale which makes design and analyses of AEM-based fuel cells and CO_2 electrochemical conversion reactors challenging. The structure and properties of these materials are dependent on both the chemistry and structure of the polymers and the solvents used to make the catalyst inks for the fabrication of electrodes.

Research strategy

This project will help understand how to manipulate the ionomer-catalyst interactions and to quantify the nanometric-scale structure and properties of the ionomers as a function of ionomer chemistry and structure, substrate (catalyst and catalyst support) and solvent. The knowledge generated will be directly applied to the design of high-performance membrane electrode assemblies for AEM electrochemical devices including AEM fuel cells for the electrochemical CO_2 electrochemical reactor. The work directly feeds into the tremendous progress the research group has made by achieving high performance more than 150 milliamperes per square centimeter (mA/cm^2) and high faradaic efficiency (more than 95 per cent) for conversion of gaseous CO_2 into CO in an alkaline exchange membrane CO_2 electrochemical conversion reactor.

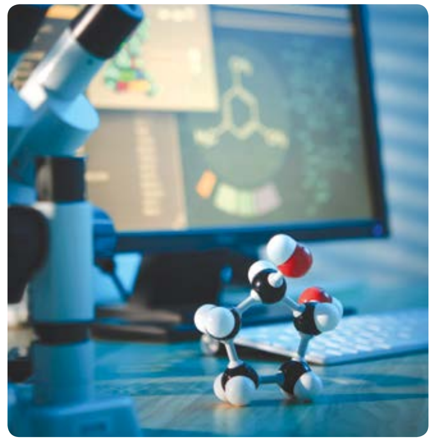
Desired outcomes

The research group is aiming to achieve high-performance CO_2 electrochemical conversion and AEM fuel cells. For the CO_2 electrochemical conversion reactor, the goal is to double the performance (from 150 mA/cm^2 to 300 mA/cm^2) by June 2019. For AEM fuel cells, the teams aim to demonstrate a high performance fuel cell (more than 1000 mA/cm^2) by late summer 2019. In addition, they will examine, in parallel, new AEM materials for carbonate transport, which can then lead to a room-temperature CO_2 separator — this will be an entirely new paradigm.

Next generation fuel cell and CO_2 separators based on anion exchange ionomers

Udit Narayan Shrivastava

Postdoctoral Fellow



Introduction

Ionomers are ion-containing polymers that are the key material component of polymer electrolyte-based devices such as fuel cells, water electrolyzers and CO_2 electro-reduction reactors. In the electrodes of these devices, the ionomers exist as thin films, nanometres thick, whose structure and properties are poorly understood. Dr. Udit Shrivastava, PhD, is working on ultra-thin ionomer films (less than 15 nanometers), measuring their transport properties and characterizing their structure and interfacial interaction with the substrate. Interfacial interaction is a key focus of this study because macro-structure of ionomer thin films depends on it, to transport properties. A major challenge is probing interfacial interaction between an ionomer thin film and a substrate and its effect on gas and ion transport the length scale is very small (approximately one nanometer). He is trying to build a structure-property relationship to assist the polymer electrolyte community develop a high performing polymer electrolyte. In addition, results from this study will guide modelling efforts.

Results

Udit has tested conductivity, water uptake and local structure (water domains within ionomers) of a variety of ionomer thin films on different substrates. An exciting finding from his recent effort is from the study of the effect of interfacial interaction between ionomer thin films and electrochemically-relevant substrate platinum (Pt) on a bulk structure. In one study with the help of neutron reflectometry (NR), he has observed that the water content at the Pt-ionomer interface depends on the length of the side-chain of the ionomers. In another study combining neutron reflectometry (NR) and grazing incidence small angle X-ray scattering techniques, he has found that the interfacial interaction between ionomer and Pt can induce non-uniform distribution of water domains (less than 1 nanometer) in ionomer thin films.

Conclusions

Interfacial hydration of three different ionomers supported on electrochemically active substrate (platinum) has been reported for the first time.

Hydration extent at ionomer/Pt interface depends on the molecular structure of the ionomer, specifically the length of the ionomer side-chain.

The results of Udit's study shows for the first time that the interfacial water and structure can be manipulated by designing different side-chain lengths.

His results have created a new awareness about the potential of controlling interfacial proton transport and electrochemical kinetics by controlling the interfacial hydration level.

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 inter-particle 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 allows 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

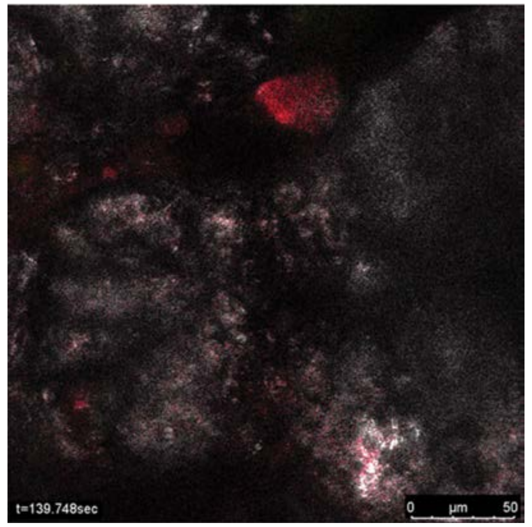
This project is creating new classes of complex fluids with tailored nanoparticles and developing novel imaging techniques that reveal how these fluids behave.

- 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

Aigerim S. Meimanova
PhD student

CNC suspension (red) plug in porous media



Introduction

As a part of this project, Aigerim Meimanova is studying the complex fluid-flow and how it is affected by the introduction of nanoparticles. The characterisation is performed through the pressure and effluent analysis in combination with the visual observation under confocal microscope. The microfluidic model compatible with the confocal microscope is already designed and used to study flow under moderate pressure.

Results

With the porous media micromodel, Aigerim has been able to identify the events corresponding to the pressure oscillations, specific to the nanoparticle-stabilized emulsion flow through porous media. Since the constituent components of the system can be tagged, the contributing effect of each can be observed. Extending this research to correlate with particle loading, flow rate hysteresis, the corresponding pressure ranges and frequency of fluctuations would allow to better understand and design fluid systems containing particles.

Conclusions

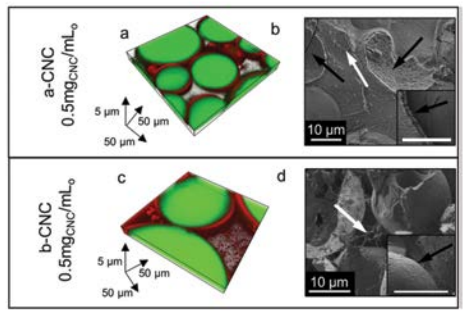
- Nano-fluids (emulsions, suspensions, foams) have a signature pressure oscillations trend when flowing.
- Micromodelling allows researchers to visually observe and analyze the effects detected with pressure fluctuations.
- The smaller size of the model (compared to common core holders) makes these effects more pronounced.

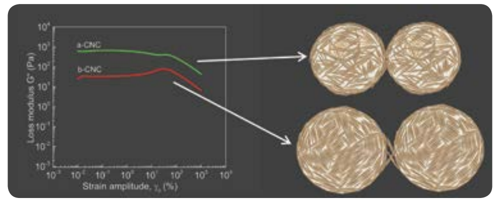
Engineered interfaces for advanced energy materials

Aseem Pandey
MSc student

Introduction

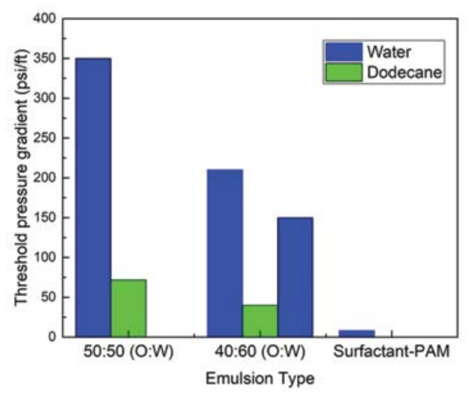
This project aims to investigate the effect of particle-particle interactions on the microstructural and rheological properties of cellulose nanocrystal (CNC) -stabilized emulsions. The fundamental understanding of the emulsions is then applied to explore their applications for conformance control in porous media. The major challenge here is to establish a precise link between the microstructure and the rheology of these complex fluids. A thorough experimental assessment of these features is of great interest to have a precise engineering control over their formulation for a wide host of technologies.





Results

Through this research Aseem Pandey established a precise link between the microstructure and rheology of the CNC-stabilized emulsion using confocal microscopy, cryo-transmission electron microscopy (cryo-TEM) and oscillatory shear rheology. He showed that the particle-particle interactions affect the morphology of the emulsions and flow-induced rheological transitions in the emulsions. As a whole, the CNC can form a strong network by droplets where particles at the droplet interface interact with each other and with particles in the bulk phase. The strength of this network is governed by the interparticle interactions and is quantified using oscillatory rheology. During the initial phase, 3D imaging of these multiphase mixtures using confocal microscopy has been cumbersome due to the abundance of scattering surfaces and required optimization of imaging parameters. However, getting a fine spatial resolution with cryo-scanning electron microscopy (cryo-SEM) has been made possible by Aseem's collaborators at Technion.



Conclusions

- Particle-particle interactions affect the final morphology of the CNC-stabilized emulsions.
- Shear-induced rheological transitions in emulsions are a function of particle-particle interactions.
- These yield stress fluids can be used for conformance control and require a very high threshold pressure for water to break through.

TECHNION RESEARCH COLLABORATION

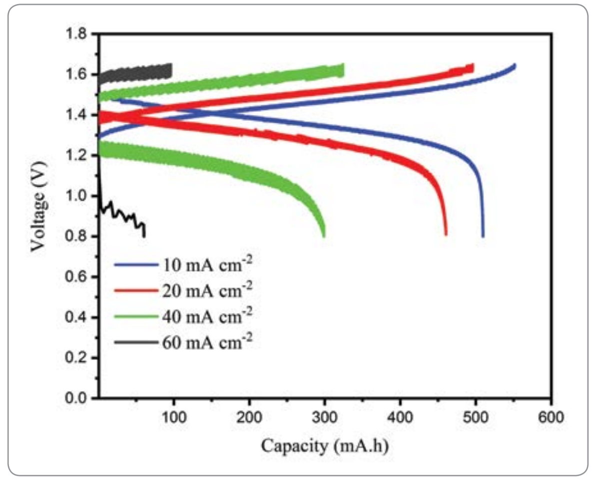
Aseem Pandey acknowledges the support of Alberta Innovates-Technology Futures and CMC microsystems.

Engineered interfaces for advanced energy materials

Farbod Sharif
Postdoctoral Fellow

Introduction

Electrodes play an important role in vanadium redox flow batteries since electrochemical redox reactions of the vanadium species occur on their surfaces. Many studies have been conducted that concern modifying the reaction kinetics on carbon or graphite felt electrodes using surface modification, such as acid or heat treatment to enhance the kinetics and consequently the energy efficiency of vanadium redox flow batteries. Lately, graphene oxide (GO) has attracted a great deal of attention due to large surface area and the high amount of oxygen functional groups at its surface. This proposed research is aimed towards utilizing the nanomaterials (cellulose nanocrystals, chitin and graphene oxide) and stabilized emulsions as templates for porous conductive electrodes. These conductive electrodes can be tuned by adding or removing the functional groups or doping with heteroatoms such as nitrogen, sulfur or boron and they can be eventually employed in vanadium redox flow batteries.



Results

Dr. Farbod Sharif, PhD, has fabricated graphene cellulose nanofibril (CNF) aerogel electrodes using an emulsion templated technique. He analyzed the behaviour of the prepared electrodes using cyclic voltammetry, electrochemical impedance spectroscopy and chronopotentiometry. The chronopotentiometry results have shown that if the battery operates at the constant current of 10 mA /cm², the current efficiency, voltage efficiency and energy efficiency would be 95, 92 and 88 per cent respectively.
The graphene CNF electrode demonstrates promising results compared to the bare graphene, suggesting that the addition of the CNF not only strengthens the structure, it facilitates the adsorption of the vanadium species on the surface of the electrode as well. These results are comparable to treated carbon paper which is the conventional electrode for vanadium redox flow batteries.

Conclusions

More battery tests and characterizations need to be performed, however based on the obtained results, the following can be concluded:

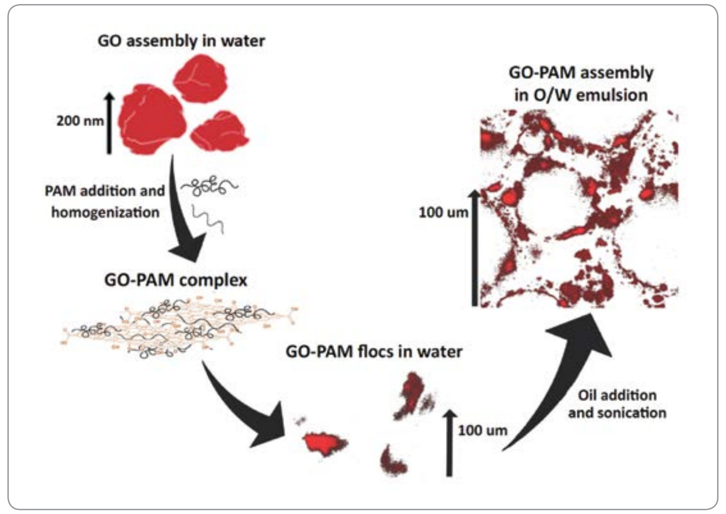
- The addition of the CNF to the aerogel enhances the mechanical strength.
- The addition of the CNF to the aerogel increases the catalytic activity for vanadium species.
- A CNF/graphene electrode has more interconnected pores leading to lower mass transfer overpotential in the battery.

Engineered interfaces for advanced energy materials

Heidi Jahandideh
MSc student

Introduction

Incorporation of nanoparticles and co-stabilizing agents are known to enhance emulsification of oil in water systems and their mechanical properties and stabilities at extreme conditions. The underlying fundamentals as to why that is the case are unclear to the scientific community. To address this issue, Heidi Jahandideh, through her master's project has designed and developed an emulsion system stabilized by mixtures of graphene oxide (GO) and polyacrylamide (PAM) as her model system to study.



Results

Heidi has observed that the emulsions stabilized by mixtures of nanoparticles and polymers are more stable under flow conditions and so can be utilized in applications such as enhanced oil recovery, drug delivery and cosmetics where emulsion systems need to remain stable under shear. In addition, the amount of nanoparticles needed to form a stable oil-in-water emulsion is significantly reduced owing to the synergistic interactions between nanoparticles and polymers.
Her research findings have been published in the peer-reviewed journal, *Langmuir.*

Conclusions

- Heidi has developed a reproducible method for correlating intermolecular interactions and microstructure to the bulk properties of emulsions and to overall emulsion stability under dynamic conditions using rheology.
- She has prepared resilient nanoparticle (NP)-polymer complexes by interfacial adsorption of polymer chains to NP's surface area via strong intermolecular forces using GO nanosheets and PAM as model materials.
- She has thoroughly investigated PAM adsorption on GO surfaces on the nanoscopic scale through atomic force microscopy (AFM), cryo-transmission electron microscope (cryo-TEM) and laser scanning confocal microscopy in GO-PAM dispersions as well as their emulsion systems.
- Utilization of GO-PAM complexes in stabilization of oil-in-water emulsions with a remarkably low GO concentration owes to the presence of PAM as a co-stabilizing agent and results in synergistic interactions.
- The use of PAM enables stabilization of GO-based emulsions at the basic pH conditions.

Engineered interfaces for advanced energy materials

Stephanie Kedzior
Postdoctoral Fellow

Introduction

Dr. Stephanie Kedzior, PhD, and her team are working on designing and fabricating emulsion-templated aerogels for battery and water purification applications. By applying her understanding of Pickering emulsions, Stephanie aims to template functional materials that can be used in a variety of applications based on the type of nanoparticles incorporated into the template.

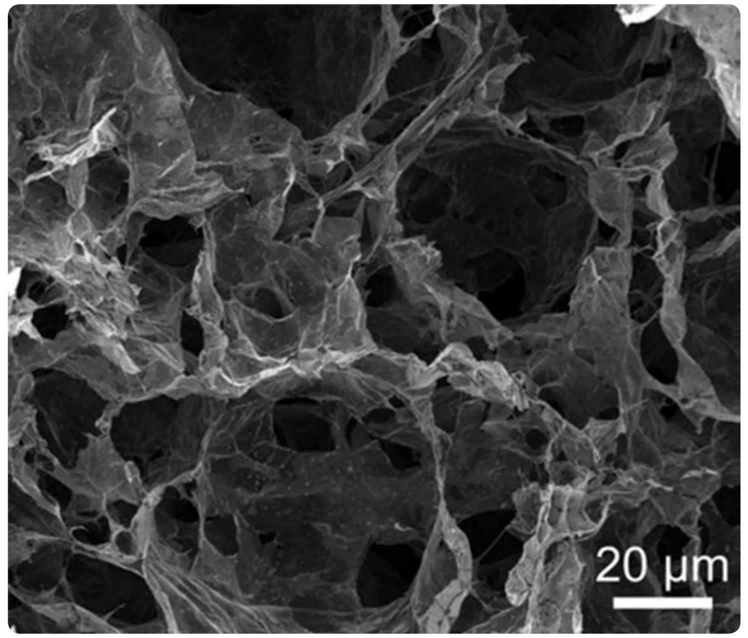
Results

To date, Stephanie has templated aerogels using cellulose nanocrystals and cellulose nanofibers with graphene oxide. The emulsion properties have been characterized using confocal and rheology microscopy and the aerogels have been characterized with scanning electron microscope (SEM). She has also tested the performance of these materials in vanadium redox flow batteries and they show potential to be used as electrodes.

Conclusions

The emulsion-templated aerogels show better performance than the treated carbon paper that is traditionally used.

The electrode porosity and structure can be optimized to provide new alternatives to traditionally used electrodes with a significant fraction of bio-based materials.



Engineered interfaces for advanced energy materials

Varvara Gordeeva
Postdoctoral Fellow

Introduction

In this project, Dr. Varvara Gordeeva, PhD is investigating the oil-in-water emulsion droplets theoretically in their hydromechanics. The goal is to find the main mechanism of interaction between the emulsion droplets by establishing a new model where the droplets are grabbed using optical tweezers. The main challenge here is that in close distance the optical tweezers begin to interfere with each other and the forces of the double optical tweezers are thus not predictable. The model will give a new tool of simulation for the droplet-droplet interaction using double optical tweezers.

Results

Varvara has observed that the challenge consists of two parts: the first part is connected with droplet-droplet interaction, the second is connected with the optical tweezers which can interfere with each other and change their properties depending on the trapped object. The interaction between the droplets can be produced by the matter of the droplets (van der Waals force), by surfaces of the droplets (electrical double layer force) and corrected with a medium between the droplets (hydrostatic pressure). Also, the optical tweezers act with additional (optical) force on the droplets trapped. All these forces are considered in developing a model of the droplet-droplet interaction. Presently, the model is at the testing stage of development. The model does not consider the interference between the optical traps at their vicinity. The properties of the optical tweezers (optical force, stiffness constant) are taken from the experiment.

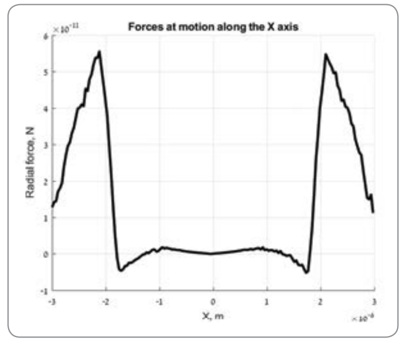


Figure 1

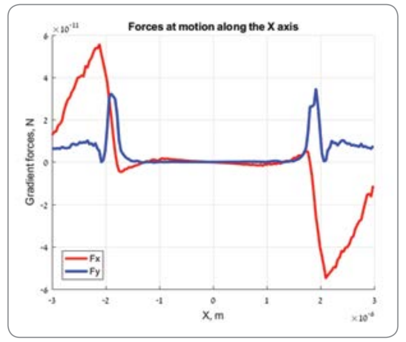


Figure 2

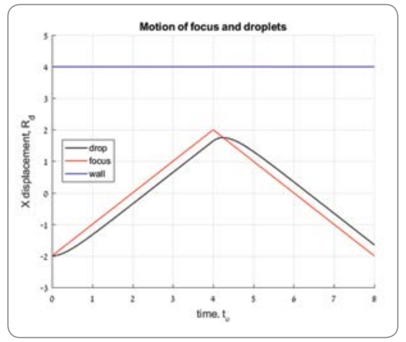


Figure 3

Conclusions

The model simulates the interaction between droplets of a liquid suspended in another non-miscible liquid and held using optical tweezers.

The optical force is calculated numerically using the Matlab package and is found to be linear in distance not exceeding the trapped object's radius (Figures 1 and 2).

The model also simulates the simplest case of hard spheres (non-deformable droplets) with no interaction between them (Figure 3).

In the next stages of the model development, the following interactions between the hard spheres will be considered: van der Waals force, hydrostatic pressure from the liquid between them and repulsion because of the electric double layer on their surface. The simulation model is made using Matlab, with properties of toluene droplets in de-ionized water.

ALKALINE METAL-ORGANIC REDOX FLOW BATTERIES FOR ENERGY STORAGE

UCalgary Team: **Edward (Ted) Roberts** • Technion Team: Dario Dekel

Background

One of the most promising technologies for energy storage is redox flow batteries. An important design parameter for a battery is the energy storage capacity, and in most batteries this is in a fixed ratio with the battery power. In this case of redox flow batteries, the materials can maintain capacity over more than 10,000 cycles, and the electrolytes are 100 per cent reusable at the end of life. However, further work is needed to enhance the power density of redox flow batteries to reduce their cost. Membrane and electrode materials, as well as the electrolyte system, are critical in this respect. The aim of the research is evaluation of different membranes, in particular cation and anion exchange materials, for redox flow batteries. Different membranes are being evaluated under a range of operating conditions in redox flow batteries.

Research strategy

The research strategy is to investigate the potential of replacing the expensive cation exchange membrane with a lower cost anion exchange membrane, and investigate the effect on the battery performance. It has been estimated that almost 50 per cent of the total cost of the redox flow battery hardware is on the cation exchange membrane (typically based on a sulfonated fluoropolymer such as Nafion). After characterizations of membranes such as ion exchange capacity, area specific resistance, conductivity and permeability, the project team found that the anion exchange membrane had the highest ion exchange capacity of the membranes as compared to Nafion. Higher ion exchange capacity leads to higher conductivity as more active sites are available for ion transport. Testing membranes in a redox flow battery system showed that at higher current densities an anion and cation exchange membrane has a very similar efficiency. Comparison between different cell designs, including inter-electrode spacing and flow rate of the electrolyte have been found to have a big impact on energy efficiency.

Desired outcomes

The project team aims to replace the expensive cation exchange membrane with a lower cost anion exchange membrane. The cycle performance of the battery may be improved with reduced cross-over of metal ions and self-discharge of the redox flow battery. Results to date have confirmed that the battery efficiency can be maintained while reducing self-discharge. The plan is to test the redox flow battery at higher current densities and run durability tests with duration up to 100 hours. COMSOL software simulations will help determine the effect of membrane properties on the charge-discharge performance.

Alkaline metal-organic redox flow batteries for energy storage

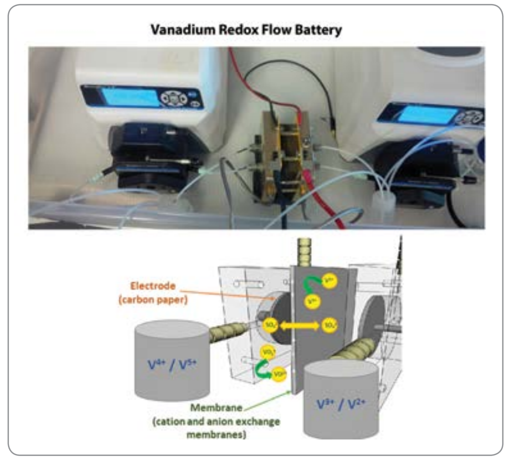
Sladjana Maslovara
Postdoctoral Fellow

Introduction

Dr. Sladjana Maslovara, PhD, is testing cation and anion exchange membranes in redox flow batteries. She is testing commercially-available anion and cation exchange membranes using a sulfate vanadium redox flow battery system under a wide range of operating conditions. The main challenge here is the long duration of the charge and discharge cycle. It takes one week for two cycles of charge and discharge with one membrane. The possible impact of the research will be to replace expensive cation exchange membranes with cheaper anion exchange ones, which will decrease the operational cost. Using anion exchange membrane in the redox flow battery will prevent self-discharge.

Results

The main outcomes of Sladjana's research were characterization (the ion exchange capacity, area specific resistance, conductivity and permeability) and testing of different membranes in a redox flow battery. She has found that a thicker membrane, such as Nafion 117, has a lower permeability of vanadium ions compared to thinner ones. Also, an anion exchange membrane with the same thickness like Nafion 212 has a lower permeability of vanadium ions which means that Nafion could be replaced. She has tested both types of membranes in the redox flow battery. The performance of the battery for charge and discharge has been determined for a range of current densities. On the higher current densities, anion and cation exchange membranes have a very similar energy efficiency. Comparing zero gap cell and cell with a two millimeter inter-electrode gap has shown that decreasing the distance between electrodes had improvement of energy efficiency of 24 per cent which directly decreases the operational cost.



Conclusions

Sladjana has done a thorough comparison between cation and anion exchange membranes in the redox flow battery. In addition to being cost-effective, replacing the expensive cation exchange membrane with the four times less expensive anion exchange membrane will prevent self-discharge of the battery.

A model of battery charge-discharge performance has been developed.

A new composite membrane has been prepared with graphene.

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, Zhangxing (John) Chen, David Eaton, Ian Gates, Steve Larter, Bernhard Mayer, Cathryn Ryan, Shengnan (Nancy) Chen, Hossein Hejazi, Haiping Huang and Kristopher Innanen.

MODELLING AND SIMULATION OF HYDRAULIC FRACTURE NETWORK GROWTH

Zhangxing (John) Chen, Shengnan (Nancy) Chen

Background

A combination of multistage hydraulic fracturing and horizontal wells has become a widely used technology in stimulating unconventional tight and shale reservoirs in the Western Canadian Sedimentary Basin. In these reservoirs, tons of fracturing fluid and proppants are pumped into the reservoir matrix to create hydraulic fractures, and economic production rates can be achieved after fracturing fluid flowback. It is important to understand hydraulic fracture propagation mechanisms, hydraulic fracture network growth, effects of their properties and controlling factors affecting flowback recovery.

Research strategy

In this project, a parallel control-volume multiphase, multicomponent, dual porosity-dual permeability (DPDK) simulator has been developed and iteratively coupled with a finite element method-based mechanical simulator to solve the coupled flow stress equations and validate the DPDK simulator with experimental data. The project team modeled *in situ* natural fracture conductivity and accounts for surface roughness and closing stress. Moreover, they produced a geologically and geo-mechanically representative fracture network map and optimized well after-stimulation operations to lead to a higher recovery factor and net present value (NPV) in unconventional reservoirs.

Desired outcomes

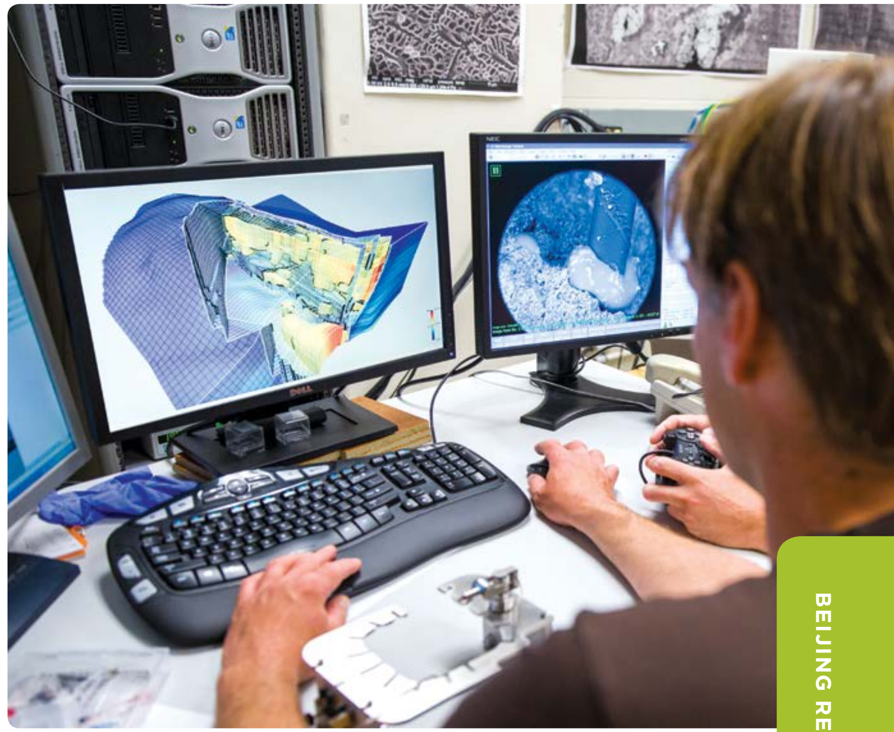
The project team anticipates building a DPDK model with numerical multiple interacting continua algorithms for a complex fracture network and a fully coupled flow and poroelastic solver for a fracture network model. Also, field-matched numerical examples on hydraulic fracture deformation will be created along with data from analysis of core samples and generation of fracture networks. New conductivity models for both natural and hydraulic fractures will also be established.

Modelling and simulation of hydraulic fracture network growth

Jie (Jason) Zhan
PhD student

Introduction

From three different perspectives (hydraulic fracture characterization, multi-scale fluid flow modelling and CO_2 sequestration in shale reservoirs), Jason Zhan's project addresses one issue: how to reliably and objectively assess and forecast the shale reservoir performance with an advanced understanding of the shale reservoir specialty? Multi-physics and multi-scale issues are involved in the modelling process. He is building a novel modelling methodology and simulation platform to depict the shale reservoir specialty. The proposed methodology and simulation platform will be valuable to the prediction of shale reservoir performance.



Results

Jason has proposed a novel and practical methodology to deal with the hydraulic fracture numerical characterization. The multi-scale simulation scheme was combined with the two-way geomechanics and reservoir coupling. The quantified induced heterogeneity (sorption-induced heterogeneity and stress-sensitivity induced heterogeneity) is valuable to the production prediction of shale formations. Incorporating the apparent permeability model into GEM, a systematic study was conducted to investigate the feasibility of CO_2 sequestration in both a dry and a liquid-rich shale formation.

Conclusions

Jason has investigated shale reservoir performance from different perspectives based on a commercial simulator and in-house simulator, and at different scales, which gives valuable guidance in field applications.

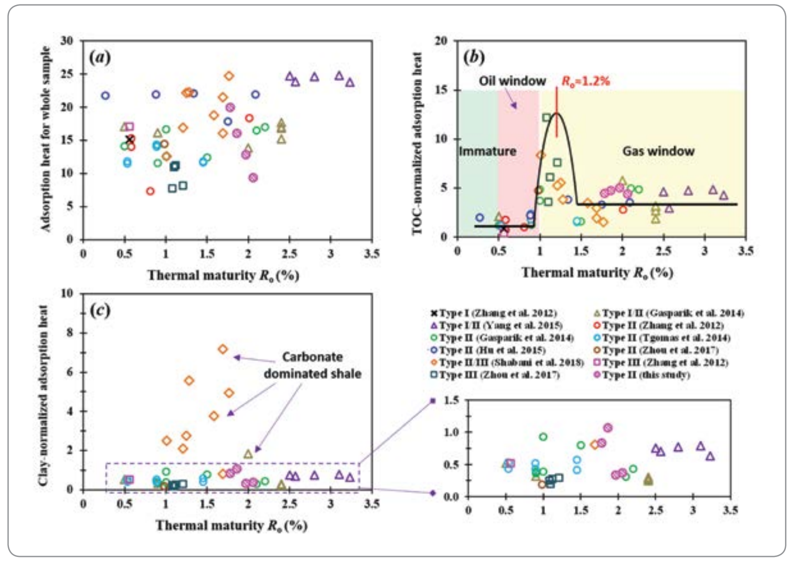
Jason Zhan acknowledges support from NSERC, Alberta Innovates, Energi Simulation Foundation, IBM Thomas J. Watson Research Center and the Frank and Sarah Meyer Energi Simulation Foundation Collaboration Center for Visualization and Simulation.

Modelling and simulation of hydraulic fracture network growth

Jing Li
Postdoctoral Fellow

Introduction

Dr. Jing Li, PhD, aims to develop a model to describe the gas storage behavior (adsorption/desorption) in nanopores and develop a model to describe the gas flow behavior (diffusion/slip flow) through nanopores. These models can be used to model storage and production of natural gas from nanoporous rocks, such as unconventional reservoirs.



Results

In the past year, Jing has established models to describe supercritical methane adsorption in shale gas reservoirs. Also, he has established models to investigate the gas slippage behavior in tight and shale gas reservoirs. Based on his research, Jing has published three journal articles.

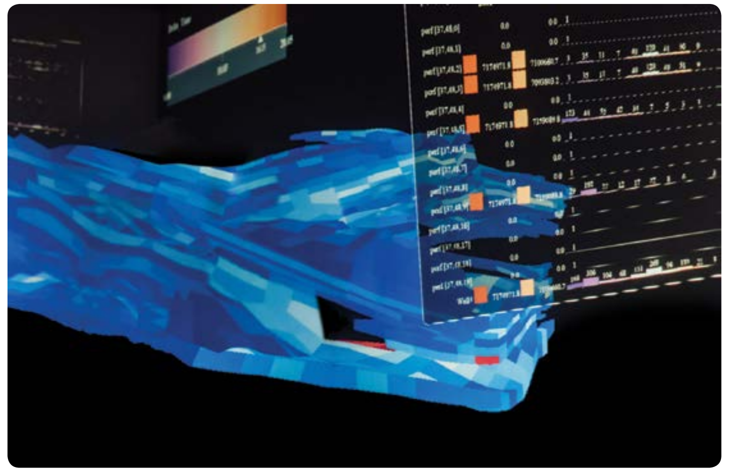
Conclusions

Jing's research provides a more accurate evaluation of gas storage and production in geologic reservoir systems.

Dr. Jing Li, PhD, acknowledges financial support from NSERC, AIEES, Energi Simulation, Alberta Innovates and the Frank & Sarah Meyer Foundation CMG Collaboration Centre.

Modelling and simulation of hydraulic fracture network growth

Ran Li
PhD student



Introduction

Ran Li has established models to investigate gas slippage behaviour during multiphase flow in shale gas reservoirs. This study puts forward an analytical model for calculating gas velocity profiles and predicting gas apparent permeability enhancement factors in shale nanopores. The proposed model considers the presence of mobile water films through modified boundary conditions. Water-gas phase behaviors was studied in shale rocks with a wide range of pore/fracture aperture size distributions. Reservoir simulation was conducted with the introduction of the previously derived gas apparent permeability model to show the gas production performance.

Results

Ran's research has indicated that ignoring a mobile high-viscosity water film tends to cause an underestimated gas velocity. The positive impacts of a mobile water film on the gas flow velocity were more significant in the case of a smaller pore size and higher pressure. Also, the Knudsen number decreased with an increase in pore size as the distance traveled by a moving molecule between two walls was increased. The Knudsen number dropped with the increase in pressure as a gas intermolecular distance is smaller and gas intermolecular collisions are more intense. A reduction in the Knudsen number resulted in a drop in the slip ratio, which is dominated by gas-wall molecular collisions. Calculations with regards to a contact angle showed that fewer hydrophilic pores possess a higher gas flow capacity. The influences from the contact angle were relatively more considerable under a smaller pore size and higher pressure.

Conclusions

In the case of smaller pores and higher pressure, a mobile high-viscosity water film was shown to make more positive contributions to gas flow.

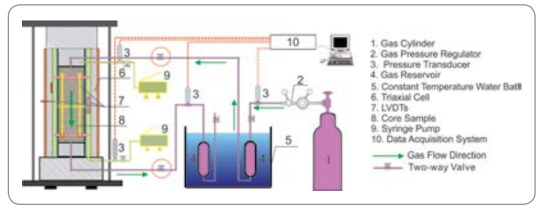
Increasing the contact angle at the solid-water interface implies the reduction of molecular attractions and the decrease of gas flow resistance.

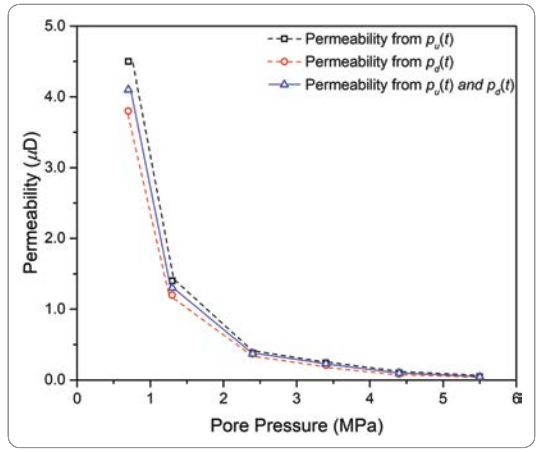
Modelling and simulation of hydraulic fracture network growth

Ruimin Feng
Postdoctoral Fellow

Introduction

Dr. Ruimin Feng, PhD, is working on the laboratory investigation of gas storage and transport mechanisms for unconventional hydrocarbon reservoir rocks. A modified pulse decay method has been proposed to accurately measure the rock porosity and permeability in the lab. Various samples will be collected to examine the gas flow behavior in rocks with different mineral compositions. Ruimin will investigate how gas flow behavior is affected under different stressed conditions, and test the geo-physical and geo-mechanical properties of unconventional hydrocarbon reservoir cores. The study has significant implications on enhanced hydrocarbon recovery by better understanding reservoir properties and fluid transportation mechanisms.





Results

Effect of gas compressibility on permeability measurement has been examined by the pressure pulse decay method. The experimental results have demonstrated that the gas compressibility is a crucial parameter that should be considered for the permeability calculations in unconventional gas reservoirs. It is suggested that both pressure changes in the upstream and downstream reservoirs should be used for permeability calculations to minimize the influence of gas compressibility on calculated permeability. Ruimin's study extends the applicability of the pressure transient technique and provides an effective way to accurately measure permeability of unconventional tight gas reservoirs.

Conclusions

Accurate measurements on effective sample porosity and permeability can be achieved by the single downstream reservoir pulse-decay method due to its capability of best replicating the *in situ* fluid flow behavior.

The effect of gas compressibility on pressure pulse responses in the downstream reservoir is stronger than that in the upstream reservoir, and the influence becomes pronounced at low pressures.

Rock permeability would be over/underestimated if only the pressure response in the up/downstream reservoir is used for permeability estimation. To maximally minimize the effect of gas compressibility on measured rock permeability, both pressure responses in the up- and downstream reservoirs are suggested to use for permeability estimation.

Dr. Ruimin Feng, PhD, acknowledges financial support from Mitacs Canada.

ENHANCED OIL RECOVERY FROM LOW PERMEABILITY HYDROCARBON RESERVOIRS

Steven Bryant, Hossein Hejazi

Background

It is critical that Canada, as an early participant in low permeability hydrocarbon resource development activity, provides a model for efficient, responsible development to guide nations, such as China, that on the cusp of shale gas development. Liquids-rich shale reservoirs in Canada and the US have anomalous fluid production characteristics compared to conventional reservoirs with similar fluid properties measured in the lab. There are various explanations for this phenomenon, but one of the more plausible is the alteration of fluid properties due to confinement in the nanopore spaces in shales. Further, the highly heterogeneous rock, ultra-tight matrix with micro to nano darcy ranges of permeability and low-to-no porosity, limits the efficiency of conventional displacement enhanced oil recovery (EOR) techniques. Improved understanding of the underlying factors governing fluid flow in tight matrices is critical for improving productivity from shales, but also developing enhanced recovery processes.

Research strategy

In this project, the effect of different additives including nanoparticles, surface treated nanoparticles, surfactants, gases and gas mixtures on the wettability/permeability of reservoir rock is being explored. The research team is analyzing different processes, including pulsed and cyclic, to probe the effects flow rates and pressures have on oil displacement. Also, under the scope of the project they are developing numerical models to optimize design for future experimental and scale-up work.

Desired outcomes

This project will help create new pressure volume temperature (PVT) models for crude oil-gas phase behavior analysis and will improve understanding of micro-wettability alterations by additives (including gases, chemical, and nanoparticles). The effects of pore geometry, pore wall properties and shear gradients on oil recovery and fluid and heat transport processes in tight rocks will be explored. Also, new simulation models to optimize improved oil recovery processes will be examined.

Enhanced oil recovery from low permeability hydrocarbon reservoirs

Colloidal behavior of nanoparticles in presence of external stimuli

Aref Abbasi Moud
PhD student

Introduction

Colloidal suspensions, such as conventional sand-water, water-kaolinite and water-cellulose nanocrystals (CNC, biomass based particles) suspensions, benefit from widespan usage in applications from advanced tailor-made materials to drug delivery systems. Aref Abbasi Moud is studying the response of nanoparticles that normally, due to negative charge on their surface, do not settle easily. Addition of polyacrylamide into kaolinite-water suspension aids settlement of kaolinite particles into bottom of the suspension. Polyacrylamide adsorbs on the edges of particles and ties them together. CNCs, on the other hand, are rod-shaped particles that do not settle due to their negative charge and tiny size. With the addition of salts, an atmosphere can be created that reduces repulsion between CNCs and causes them to adhere to one another in the form of gels. Challenges faced so far are adjustment the timing of gelation and controlling porosity of the gels.

Results

In this study, Aref has observed that the addition of counter ions, either magnesium chloride ($MgCl_2$) or sodium chloride (NaCl), causes sudden phase separation in CNC-salt hybrid systems. This means that CNCs adhere to one another and come out of the phase of water. It has also been witnessed through theoretical observations that the structures are self-similar. This means that structure from the micro-size scale replicates itself until it becomes large enough to cover the whole visualization cube. Confocal laser scanning microscopy micrographs complemented information obtained via transmission electron microscopy (TEM), which depicts their power in monitoring colloidal behavior of CNC suspensions. Particles were found to adhere into structures that were stickier at lower concentrations of salt. Derjaguin, Landau, Verwey and Overbeek (DLVO) theory also has been used to predict colloidal behavior of CNCs. Based on the values found, this theory predicts at what salt concentration a phase separation is likely to to seen. CNC gel has also been found to be more resistant towards the effect of gravity when the structure is formed out of more concentrated CNC suspensions.

Conclusions

- Aref investigated the colloidal behavior of CNCs with confocal microscopy under the influence of NaCl. Experiments have shown that when using confocal microscopy, the rate of gel collapse can be measured as a function of time.
- The addition of counter ion, either $MgCl_2$ or NaCl, causes sudden phase separation in CNC-salt hybrid system.
- Calculated fractal dimensions show that salt concentration affects the morphology of the cluster in a way that at lower salt concentrations, less branchy clusters are formed.
- Gelation of CNC shows peculiar behaviors and many unique experiments have been designed.
- Kaolinite-polyacrylamide suspensions show that polymer chains adsorb on the edges of kaolinite particles.

Aref Abbasi Moud acknowledges financial assistance from Kerui- MITACS Accelerate Research Fund.

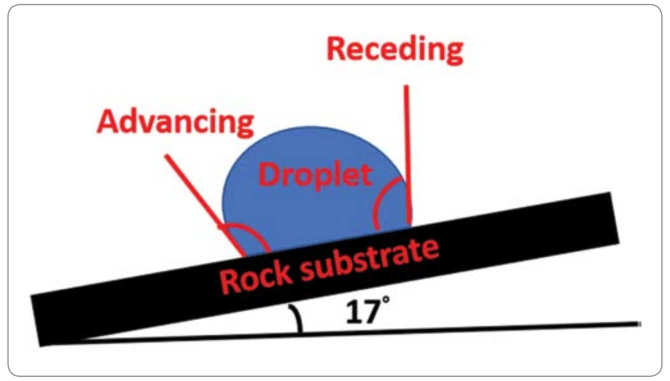
Enhanced oil recovery from low permeability hydrocarbon reservoirs

Rock surface wettability characterization through dynamic contact angle at elevated pressures and temperatures

Bin Pan
PhD student

Introduction

Oil and gas are stored in the micropores (and nanopores in the case of tight and shale reservoirs) of underground rocks. The hydrocarbon reserve estimation and recovery largely depends on the affinity of the oil, gas and water to the solid mineral surfaces in porous rock, characterized by wettability. Many parameters including types of fluids, minerals, pore sizes, pressures and temperatures can influence the wetting properties of rocks. In this project, Bin Pan studies the competition between water/gas/oil to wet the unconventional reservoir samples at high pressures (up to 30 megapascals) and temperatures (up to 70 C).



Results

The experimental results have demonstrated a strong correlation between the surface wettability of the shale rock samples to the pressure, temperature and the fraction of organic matters that forms the rock. The oil affinity to the shale samples becomes stronger when the rock contains a larger fraction of organic matters. At reservoir conditions (25 megapascals and 50 C), the strongly water-wet rock sample becomes methane-wet when the fraction of organic matters increases from 1.3 to 20.05 weight per cent. In addition, the shale samples become hydrophilic as the temperature increases. Quartz wettability correlates with the density of the non-aqueous fluid (e.g. oil, CO_2, nitrogen, etc.) — which can be in liquid, gaseous or supercritical form.

Conclusions

Higher total organic carbon (TOC) leads to stronger hydrophobicity.

Higher temperature leads to higher water-wet condition; the temperature influence is reduced at higher TOC.

High TOC shifts shale wettability from hydrophilicity to hydrophobicity.

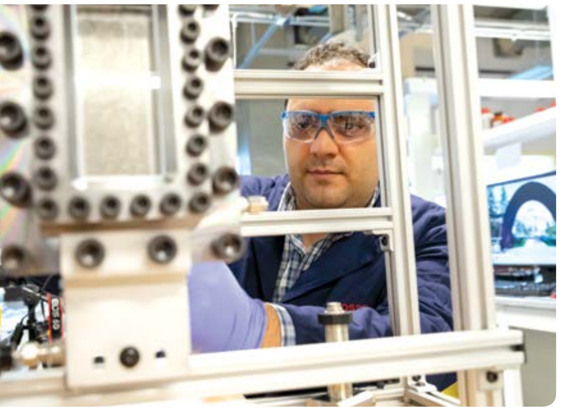
The equilibrium contact angle for a specific temperature, mineral surface and brine composition correlated linearly with hydrocarbon and generally the non-aqueous fluid density.

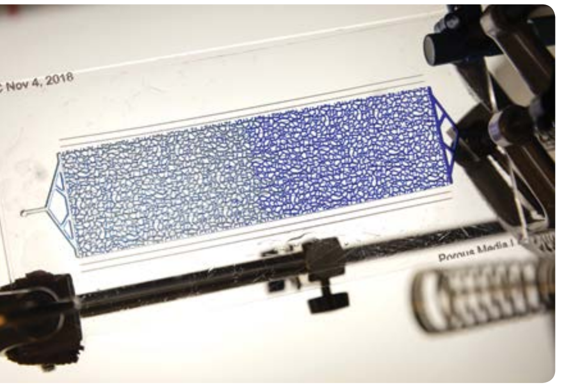
Bin Pan acknowledges funding from the Mexican partners.

Enhanced oil recovery from low permeability hydrocarbon reservoirs

Cyclic supercritical fluid soaking for enhanced oil recovery in liquid rich tight/shale resources

Hossein Khorshidian
Postdoctoral Fellow





Introduction

The research Dr. Hossein Khorshidian, PhD, is conducting is related to the development of novel techniques to improve oil production from unconventional resources beyond the current 5 per cent to 10 per cent recovery range. The challenge in unconventional resources is that oil is locked in tiny (micro- and nano-scale) pores of rock and does not flow easily. Injection of fluids that easily mix with the oil, referred to as miscible solvents such as CO_2, has shown slight increments in oil extraction from tight reservoirs. Hossein studies the coupling effect of solvent injection and pressure maintenance to minimize the effect of heterogeneities on oil recovery from a matrixed-fractured reservoir, hence, maximizing the oil extraction. His research impact will be to access more than 90 per cent of oil in tight and shale reservoirs that is currently unrecoverable using current technologies.

Results

An important step in this research is the development of a transparent porous medium where the three phase flows of oil, gas and water, including phase change, can be accurately monitored. Pore network micromodels have been used for visualizing the oil displacement, however, this is under low pressure and temperature conditions. Hossein has designed and fabricated a unique high pressure, high temperature (HPHT: 200 bars, 150 C) pore-level visualization setup that is used for displacing oil with supercritical fluids. The development of pore network micromodel is a very complex process that is in fact a combination of art and engineering. Moreover, an experimental setup including imaging system, pumps and piping instrumentations and data acquisition system has been developed for conducting experiments efficiently with minimal systematic and human errors involved. In parallel, numerical simulation is developed to examine and optimize different patterns of solvent injection in a heterogeneous medium. The preliminary results have demonstrated solvent injection schemes under which oil flows from tiny pores towards main flow paths.

Conclusions

- Hossein has designed a novel HPHT visualization vessel (200 bars, 150 C) designed and fabricated to perform pore-level experiments under reservoir conditions.
- Innovative protocols are established for the construction of pore network micromodels.
- An efficient experimental setup is prepared for conducting pore-level tests and reducing the effect of uncontrolled parameters on the quality of data.
- Numerical simulation is developed for studying the effect of fluid injection pattern on the oil displacement efficiency.

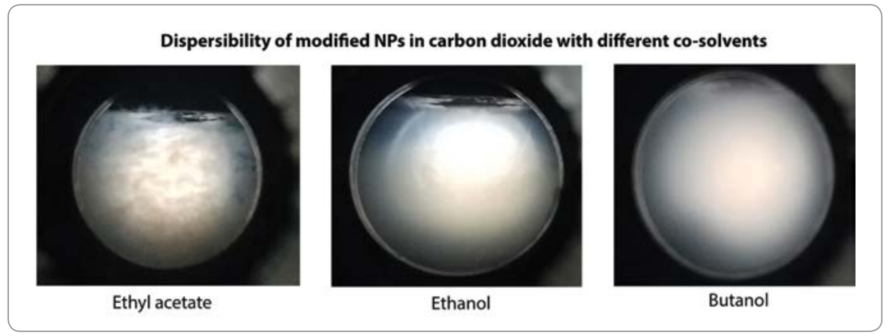
Enhanced oil recovery from low permeability hydrocarbon reservoirs

Transport of nanoparticle-stabilized foams and emulsions for improved oil recovery

Qian Sang
Postdoctoral Fellow

Introduction

The main goal of Dr. Qian Sang's project is to find a system using nanoparticles to increase the viscosity of CO_2. The biggest challenge is to disperse nanoparticles (NPs) in CO_2. Therefore, she grafts polymer chains on the surface of the nanoparticle to increase its ability to disperse in CO_2 and evaluates the phase behavior and viscosity of NPs-polymer-solvents systems. Dispersing NPs into bulk phase CO_2 has not been previously reported, so even the small concentrations achieved in this project is an important step forward.



Results

In this study, Qian used poly(vinyl acetate) to modify the surface of nanoparticles to increase their dispersion in CO_2. She has found a suitable solvent to disperse the polymer modified nanoparticles in CO_2 and increase the viscosity by two to three times. However, the dispersibility of the system is limited and the viscosity is still lower than desired for fracture stimulations. Also, large concentrations of the solvent are usually required, and the concentration of dispersed nanoparticles is still smaller than the values needed to increase viscosity in other fluids. Thus the goals have partially been achieved. It is still necessary to continue to modify the nanoparticles to further increase the viscosity for the target applications.

Conclusions

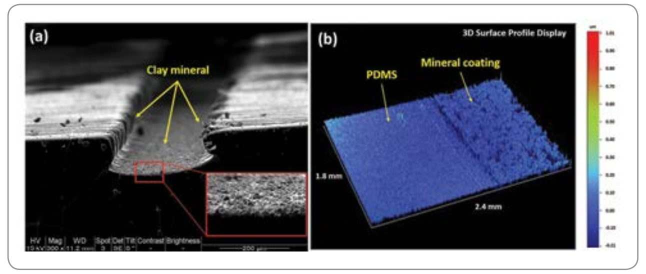
- Qian has developed a NPs-polymer-solvent system suitable for dispersing NPs into supercritical CO_2.
- Experimental results of phase behavior and viscosity for a range of temperature, pressure and composition have been obtained for this system.
- Apparatus for making these measurements has been set up.

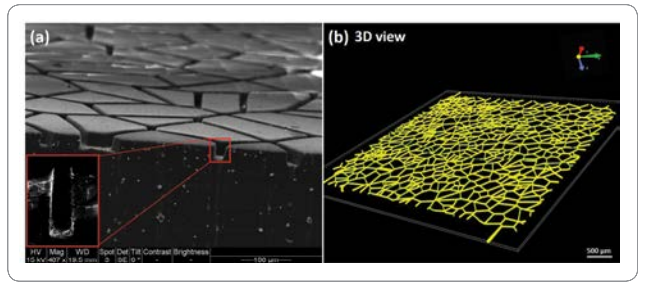
Dr. Qian Sang, PhD, acknowledges the support of Mitacs-Accelerate Project, Discovery Grants of NSERC and China University of Petroleum (East).

Enhanced oil recovery from low permeability hydrocarbon reservoirs

Development of geomaterial-based microfluidic devices for oil and gas applications

Yaqi Zhang
PhD student





Introduction

Yaqi Zhang's aims to develop surface-mimetic micro-reservoir (SMMR) platforms which are used for studying enhanced oil recovery (EOR) problems. Different surface treatment methods are employed to modify conventional micromodels and a proper method is selected to functionalize conventional micromodels with realistic rock surface properties. The developed surface-functionalized micromodels overcome the shortage of using synthesized microfluidic devices — lacking realistic rock surface properties. By the developed SMMR platforms, EOR and reservoir stimulation processes relevant to fluid-rock interactions can be examined cost-effectively and quickly before any core-scale study and field implementations.

Results

The output of this work has been a series of custom-built SMMRs, which have potential applications for subsurface energy and environmental issues, including various EOR projects. These devices are especially advantageous in studying phenomena related to fluids-rock interactions, such as the effects of nanoparticles, surfactants and polymers in reservoirs.

Conclusions

- A novel technology of functionalizing micromodels with geomaterials has been developed.
- This work develops robust microfluidic platforms which involve SMMRs.
- By using the developed SMMR platforms, geological processes such as EOR techniques and geological storage can be visually investigated. Especially, fluid-rock interactions can be studied.

Yaqi Zhang acknowledges NSERC, the China Scholarship Council (CSC), the CMC Microsystems and the Canada Foundation for Innovation.

Enhanced oil recovery from low permeability hydrocarbon reservoirs

Zehao Yang
PhD student

Introduction

The presence of suitable nanoparticles (NPs) at certain concentrations within a liquid phase increases the diffusivity of solutes in that liquid. Zehao Yang seeks to exploit this property to increase the rate of transfer of a component between a liquid phase and a second fluid phase. Such transfers can enhance the flow properties of one phase. Zehao's plan is to conduct experiments at elevated temperatures and pressures with fluids contained in porous media and in vessels or channels. The experiments will be at two length scales: centimeter-scale cores and sand packs, and micron-scale channels in which menisci can be observed directly.

Results

Zehao has shown that diffusivity within the nanoparticle-containing fluid exhibits a clear maximum as nanoparticle concentration increases. His research has also demonstrated that by using a commercial nanoparticle dispersed in water, the maximum mass transfer enhancement in a gas/water system is 20 per cent at the concentration of 0.08 weight per cent nanoparticles. Also, using magnetite nanoparticles under a direct current magnetic field, the mass transfer has been shown to increase tenfold. Mathematical models have shown that resistance to mass transfer at the gas/liquid interface is small compared to the diffusive resistance. When the concentration of NPs is high, the mass transfer has decreased, the determination of optimum concentration remains obscure. CO_2 dissolution into water is important for carbon capture and storage applications, but this results in convection currents in the centimeter-scale setup. Zehao is planning to pursue these experiments in collaboration with Tsinghua University.

Conclusions

- Nanoparticles dispersed in liquid increases diffusivity within that liquid but only up to a critical concentration. Above this concentration, the diffusivity decreases.
- A magnetic field may greatly enhance diffusivity within liquid containing magnetite NPs.
- The pressure-decay method is convenient for inferring mass transfer parameters both at the interface and within a fluid.

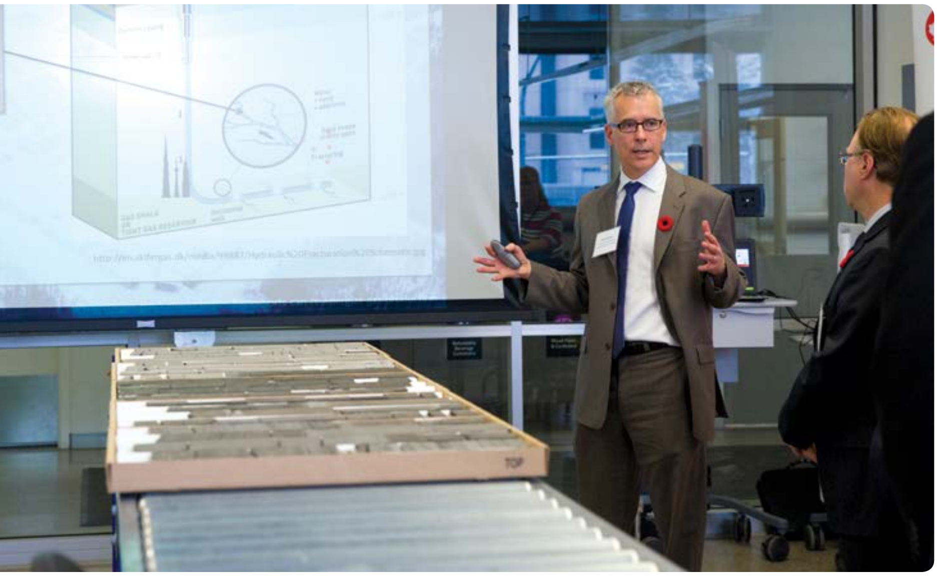
Zehao Yang acknowledges National Key Basic Research Program of China (973 Program) and Natural Science Foundation of China for funding the research.

IMPROVED SEISMIC PROCESSING FOR BETTER RESERVOIR CHARACTERIZATION

David Eaton, Kristopher Innanen

Background

Hydraulic fracturing is accompanied by brittle deformation within the reservoir that produces microearthquakes (microseismic events) that can be recorded using sensors placed in boreholes or at the surface. The recorded ground motion can be used to locate and characterize microseismic events, thus providing valuable information to image and control fracturing processes. Induced seismicity consists of earthquakes caused by human activities, such as fluid injection or withdrawal or deep underground mining. Anomalous induced earthquakes, accompanied by microseismicity, have occurred in association with hydraulic fracturing in both China and Canada. This project will extend work completed to date to analyze induced seismicity and provide a forum to exchange ideas and information between researchers at the University of Calgary and researchers in China.



Research strategy

Two approaches are being used for this research program. The first involves the development and application of advanced data processing methods to investigate microseismicity to identify low-amplitude, small-magnitude events in a noisy environment. The characteristics of such events (e.g. temporal and spatial extents, frequency content, similarity to other events) can help in understanding reservoir characteristics, develop a better understanding of how to image and control fracturing and understand the influence of human activities on the natural environment. This work takes advantage of open-source software and available high-performance computational facilities. The second approach involves detailed studies of the source mechanism for induced (human caused) earthquakes. The earthquake source mechanism, known as a moment tensor, reveals the fundamental characteristics of an earthquake that can provide important clues about the stresses within the Earth and the orientation of possible fault planes. Both projects make use of data from the Tony Creek dual microseismic experiment (ToC2ME), which was acquired using a dense, shallow borehole array to record continuous 3C waveform data.

Desired outcomes

Case studies developed using microseismic data have been applied to estimate *in situ* stress and will be applied to estimate stimulated reservoir volume (SRV) dimensions through the analysis of a high-quality event catalogue derived using innovative processing methods. This research project will ultimately contribute to the development of a rock physics model which considers effects of attenuation, anisotropy and stress to study how fractures and fluids affect the stiffness matrix of a gas-bearing fractured rock.

Improved seismic processing for better reservoir characterization

Ali Fathalian
PhD student

Introduction

Simulation of wave propagation in a constant-Q viscoacoustic medium is an important problem, for instance within Q-compensated reverse-time migration. Processes of attenuation, dispersion and anisotropiy influence all aspects of seismic wave propagation, degrading resolution of migrated images. To improve image resolution, Ali Fathalian presents a new approach of the viscoacoustic wave equation in the time domain to explicitly separate amplitude attenuation with phase dispersion and develop a theory of viscoacoustic reverse time migration (Q-RTM) in tilted transverse isotropic (TTI) media. Because of this separation, it would be possible to compensate for the amplitude loss effect, the phase dispersion effect or both effects.

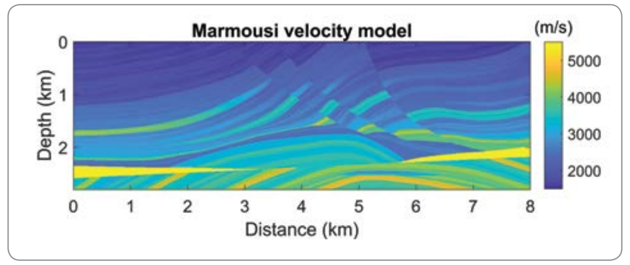


Figure 1

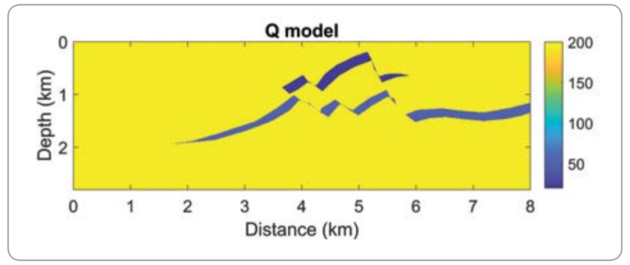


Figure 2

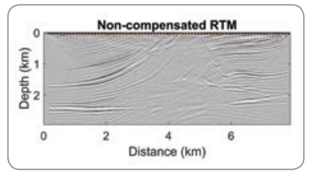


Figure 3

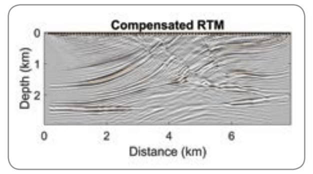


Figure 4

Results

To demonstrate the effect of attenuation, Ali has applied viscoacoustic RTM to the viscoacoustic data set to generate the Q-RTM image in TTI media. The amplitude loss and phase dispersion in the receivers' wavefields can be recovered by applying compensation operators on the measured receiver wavefield. Ali has tested a new approach to the complex Marmousi model (Figure 1) with a Q anomaly (Figure 2). In acoustic RTM with viscoacoustic data (noncompensated RTM) (Figure 3), there are some regions with amplitude loss and shifted phase due to velocity dispersion. The high-attenuation anomaly causes a reduction in wave amplitude, so migrating the attenuated data produces the weak reflectors. To solve the poor illumination problem of viscoacoustic RTM images, he has applied for attenuation compensation during wave propagation using the new Q-RTM approach. The compensated image (Figure 4) indicates improved RTM image with recovered amplitudes of the reflectors at the dip depths.

Conclusions

Ali has presented a methodology of Q-RTM in anisotropic media that is able to mitigate dispersion and attenuation effects in the migrated images.

The amplitude loss and phase dispersion in the source and receivers wavefields can be recovered by applying compensation operators on the measured receiver wavefield.

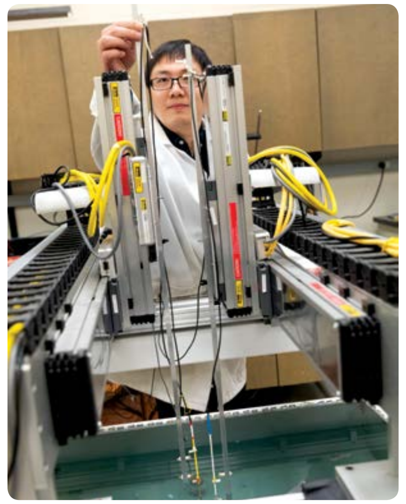
Ali Fathalian acknowledges support from NSERC and Mitacs.

Improved seismic processing for better reservoir characterization

Hongliang Zhang
PhD student

Introduction

With the aim of understanding the source-mechanism variability and local stress environment near the Fox Creek area, Hongliang Zhang has undertaken detailed investigations of induced seismicity during a four-well hydraulic-fracturing completion program. This project makes use of data from the Tony Creek dual microseismic experiment (ToC2ME), which has been acquired with the use of a dense, shallow borehole array to record continuous 3C waveform data. In addition to unusually good azimuthal coverage, this array enables a significantly lower magnitude of completeness than regional monitoring networks. Here, 3C geophone data for high-quality events are used to estimate moment-tensor solutions and local stress field.



Results

Based on the moment-tensor solutions for 530 high-quality events, in addition to the previously documented north-south/east-west trending strike-slip mechanism on subvertical planes, Hongliang has identified the several other groups of source mechanisms, including strike-slip mechanism on subvertical northeast-southwest/northwest-southeast trending nodal planes and strike-slip mechanism showing either low dip angle on the northeast-southwest trending nodal plane or significant oblique dip-slip on the northwest-southeast trending nodal plane. He has used two different approaches to invert the local stress field based on a typical assumption of double couple (DC) mechanism and a recently generalized approach that assumes shear-tensile mechanisms. These two approaches yield similar results, both compatible with a strike-slip regime with maximum horizontal stress (S_{Hmax}) along the direction of approximately north sixty degrees east. This orientation differs from the median regional S_{Hmax} direction (approximately 45-47 degrees) by about 15 degrees, but is very similar to a measured S_{Hmax} direction (57 degrees) at the nearest available location in the World Stress Map.

Conclusions

Spatial distributions of induced events display clear linear alignments along either north-south or northeast-southwest direction.

Significant non-DC has been observed for one group of events.

Stress inversion implies a strike-slip regime with S_{Hmax} of about 60 degrees, and the north-south fault that produced the strongest events is not optimally oriented for slip.

Hongliang Zhang acknowledges two anonymous companies for providing access to the shallow-borehole array used for the ToC2ME project, which used the BuriedArray acquisition method used under license from Microseismic Inc.; support from NSERC; the CRD grant supported by TransAlta Utilities and Nanometrics Ltd.; additional sponsors of the Microseismic Industry Consortium; and Mitacs.

Improved seismic processing for better reservoir characterization

Huaizhen Chen
Postdoctoral Fellow

Introduction

In this project, Dr. Huaizhen Chen, PhD, focuses on the prediction of fractures and the estimation of attenuation factors from observed seismic data, in which he aims to demonstrate an approach of seismic inversion for fracture weaknesses and inverse quality factors. The challenge is how to construct a stable and reliable algorithm and workflow to implement the inversion of seismic data. His proposed approach will be a useful tool to predict fractures and fluids, which can provide additional information for reservoir characterization.

Results

Huaizhen has established a stable and reliable approach to employ surface seismic data to estimate fracture-related parameters and attenuation factors. Based on this approach, he has also proposed a detailed workflow of implementing seismic inversion using the seismic wave reflection coefficient that is derived as a function of fracture weaknesses and attenuation factors. The derived reflection coefficient can also be used as a tool for generating seismic data when given different fracture properties (e.g. fracture aspect ratio and fracture density) and fluid parameters (fluid bulk modulus and viscosity).

Conclusions

Huaizhen demonstrates a stable and reliable approach of employing surface seismic data to estimate fracture-related parameters and attenuation factors.

Applying the approach to synthetic and real data, he concludes that the proposed approach can provide additional and reliable results for fractured reservoir characterization.

Dr. Huaizhen Chen, PhD, acknowledges support from NSERC. The SINOPEC Key Lab of Multi-Component Seismic Technology is thanked for providing the processed real data.

Improved seismic processing for better reservoir characterization

Rebecca Olivia Salvage
Postdoctoral Fellow

Introduction

Dr. Rebecca Salvage, PhD, focuses on researching the development of novel techniques to investigate microseismicity associated with hydraulic fracturing activities. She aims to identify low amplitude, small magnitude events from within a noisy environment. The identification and analysis of such events (e.g. temporal and spatial extents, frequency content and similarity to other events) will allow researchers to constrain reservoir characteristics, develop a better understanding of the propagation of fractures at depth and understand the influence of human activities on the natural environment. This has become particularly important as a number of large magnitude earthquakes have been reported in relation to hydraulic fracturing.

Results

Rebecca is using techniques to identify specific signals within continuous seismic data that are often hidden by noise, and therefore overlooked. These signals, however, have the ability to seriously alter the current understanding of the location and characteristics of microseismicity at depth in relation to hydraulic-fracture experiments. She is developing methods to identify and locate microseismicity directly related to hydraulic-fracture operations, which are mostly extremely low amplitude events. The results obtained suggest that a number of sequences of repeating seismicity occur during hydraulic fracturing experiments, suggesting events occurring at similar locations and generated by similar mechanisms. Analysis of the temporal and spatial variations in repeating microseismicity offers a unique insight into the development of this highly pressurised system, in particular in relation to subtle changes in the frequency content, number of events and amplitudes of events, which would otherwise be missed.

Conclusions

Low amplitude events are often missed from analysis due to noise but are essential for a complete understanding of hydraulic-fracture experiments, in particular the evolution of seismicity in time and space.

Repeating microseismicity offers unique opportunity to study subtle changes in fracture propagation in the sub-surface.

Dr. Rebecca Salvage, PhD, acknowledges two anonymous companies for the deployment of geohones and data collection for the hydraulic fracture experiment; financial support provided by Chevron and NSERC; geophone data collected by Terra-Sine Resources and recorded under license from Microseismic Inc. for use of the BuriedArray method; additional sponsors of the Microseismic Industry Consortium; data processing and analysis conducted using Obspy and REDPy; and Alicia Hotovec-Ellis (USGS) for her unrelenting help in all REDPy matters.

ENVIRONMENTAL MONITORING OF SHALE GAS ACTIVITIES

Bernhard Mayer, Cathryn Ryan

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 shallow groundwater. To properly assess potential environmental impacts from the development of unconventional hydrocarbon resources, a detailed understanding of the chemistries of reservoirs gases, flowback fluids and produced waters from hydraulically fractured reservoirs is needed. Furthermore, a better understanding of the production and geomechanical implications of free phase methane is needed. The transport of free gas methane into shallow aquifers poses a risk for groundwater quality and rapidly increases pore pressures, which in turn could affect locally stressed faults in the geological formation.

Research strategy

In this project, the project team uses chemical and isotopic characterization of reservoir gases, flowback fluids and produced formation waters to better understand reservoir processes and generate baseline data that can be used to assess potential future environmental impacts. They also investigate whether the formation of free gas and the associated increased total dissolved gas pressures can result in decreased effective stress, free phase gas transport, over-pressuring and faulting of tight rock.

Desired outcomes

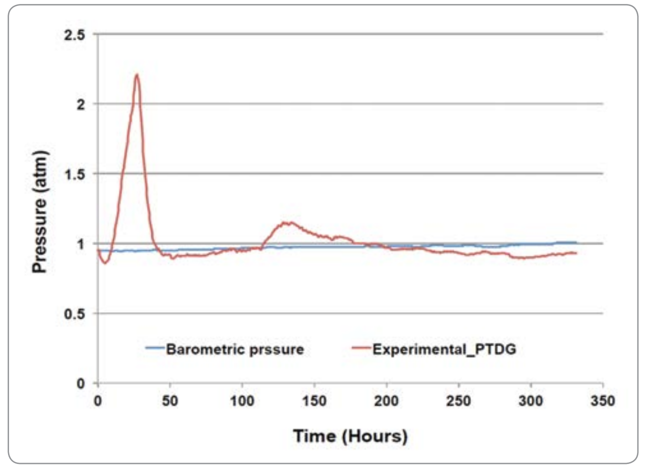
As a result of this study, the project team will be able to unravel geochemical reservoir processes and generate baseline data that can be used to assess potential future environmental impacts on shallow groundwater. In addition, the impact of pressurization on sandstones and shales through formation of a free gas phase will be better understood. Through improved understanding of the mechanisms for free gas formation and transport through tight resources, associated risk mechanisms can be better understood including failure of faults and a basin-scale understanding of potential free gas transport into freshwater zones.

Environmental monitoring of shale gas activities

Navreet Kaur Suri
Postdoctoral Associate

Introduction

Dr. Navreet Suri, PhD, is researching how to induce biogeochemical free phase gas (FPG, i.e. bubble) production to increasing dissolved gas concentrations through microbially-facilitated processes such as methanogenesis or denitrification. The goal is to generate sufficient dissolved gas to reach the bubbling point to generate *in situ* bubbles. In undrained systems, this would increase pore water pressure and decrease effective stress with consequent over-pressurization that could lead to hydraulic fracturing. In addition to supporting a graduate student's project, Navreet's work is also directly related to enhancing oil recovery by FPG production. In the case of denitrification, it can also inhibit oil field souring (i.e. by inhibition of sulfate reduction).



Results

So far, Navreet has isolated strains of denitrifiers from a nitrate reducing microbial consortium enriched from a subsurface water sample and complete reduction of up to 100 millimole of nitrate has been demonstrated. The total dissolved gas pressure (PTDG) increases from 0.88 to 2.1 atmosphere through nitrogen (N_2) formation, which overpressurizes the 120 milliliter microcosms with a headspace of 10 milliliter. Although this seems promising for enhanced oil production, it is insufficient for the proposed geomechanics research. Attempts are being made to achieve higher increases in PTDG, with a focus on methanogenesis.

Conclusions

Biogeochemical gas formation can be effectively induced to increase PTDG and produced FPG, which could be an approach for enhanced oil recovery.

Methanogenesis is being evaluated to provide a greater degree of biogeochemical dissolved (and free phase) gas production for geomechanical laboratory experiments.

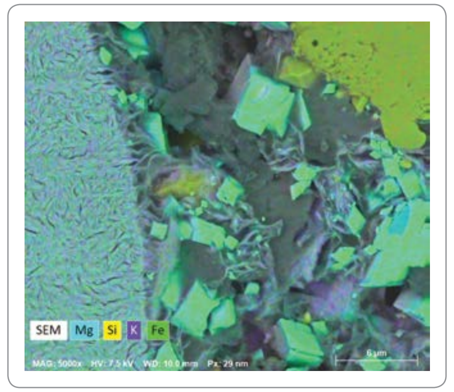
Environmental monitoring of shale gas activities

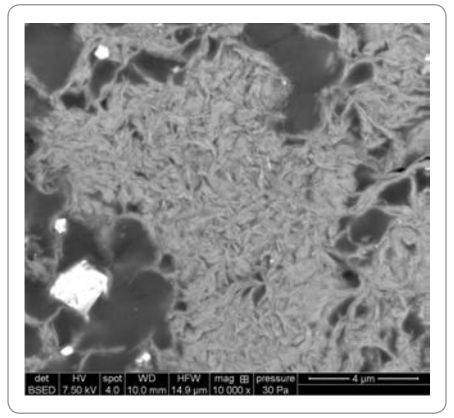
Numerical simulation of geothermal systems in Guantao Group, Shandong, China

Qin Zhang
PhD student

Introduction

Geological carbon sequestration has become increasingly relevant worldwide as many countries and industries globally are seeking ways to significantly reduce anthropogenic CO_2 emissions. Potential carbon storage sites need to be closely examined since many of the rock formations are complex and contain a variety of minerals that react with CO_2 differently. To predict the consequences of injecting CO_2 into reservoir rocks, it is helpful to study sites where natural carbon sequestration has been ongoing through geological time. These sites provide fundamental data to predict the chemical behaviors of CO_2 and guide the design of innovative experiments and large-scale carbon sequestration operations.





Results

Glauconite is an iron-rich clay mineral abundant in marine greensands worldwide. Evidence from these formations suggests that glauconite is commonly diagenetically converted to iron-carbonate minerals. This process represents a natural CO_2 sink that may provide an effective mechanism for permanent storage of anthropogenic greenhouse gases. In this study, Qin Zhang has sampled glauconitic sandstones in Western Alberta and examined their elemental composition and mineralogical properties. These observations combined with thermodynamic calculations has shown strong evidence that given the right redox, pH, partial pressure of carbon dioxide (pCO_2) and temperature conditions, glauconite carbonation should proceed to completion. While studying the natural analogues, Qin has also been designing a laboratory experiment using pure glauconite to simplify the natural system and study the behavior of CO_2 reacting with glauconite. She has encountered difficulties obtaining high quality glauconite samples, for separating glauconite from the sandstones is extremely time consuming. An electromagnet has been built to solve this problem and is being tested.

Conclusions

Greensand formations are ideal CO_2 sequestration sites because they are widespread, accessible and abundant.

Glauconite in greensands has great carbon sequestration potential given the right conditions.

This study provides fundamental data to create methods to characterize and select sequestration sites, approaches to ensure safe operation and even regulatory overview and long-term liability management.

Environmental monitoring of shale gas activities

Geomechanical implications of free phase gas production

Yuan Zhang
PhD student

Introduction

Yuan Zhang aims to evaluate the implications of free phase gas (FPG, i.e. bubble) formation in the subsurface, which is involved in natural hydraulic fracturing and subsurface gas migration, and is implicated in earthquake initiation and propagation. The goal is to promote FPG generation in a triaxial cell to the point of over-pressure and geomechanical failure. This will permit better understanding of the FPG formation process and implications for effective stress, which in turn will help to parameterize hydraulic fracturing models. To date, this research has been conducted in a uniaxial cell, where total dissolved gas pressure, water pressure, temperature and moisture content were measured under changing pressure conditions.

Results

Yuan's uniaxial cell testing has shown that by increasing the temperature, pressure changes are induced to 511 kilopascals, when FPG is formed. After four hours of equilibration, total dissolved gas pressure and pore water pressure reached a similar value. Subsequent decreases in pressure was seen mainly due to leakage from the uniaxial cell. In theory, if the cell is well sealed, pressure should maintain the same value during this period. When the temperature decreased, a delay was seen in the pressure response. This delay was attributed to the time required for diffusion of dissolved gases from the free- to dissolved-phase.

Conclusions

Early experiments have validated the equipment and uniaxial set up, and will be transferred into a triaxial cell where biogeochemical FPG production will be stimulated.

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.

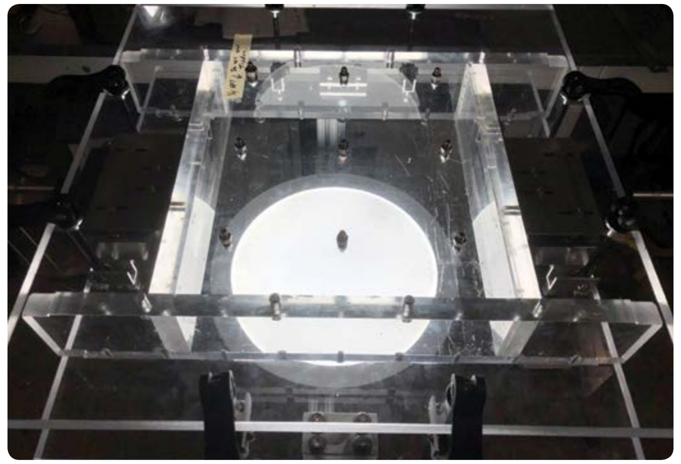
Improved and alternative energy recovery from petroleum reservoirs

The movement of proppant in a hydraulic fracture

Guangyu Shi
MSc student

Introduction

The fate of proppant in hydraulic fractures remains unclear. In this project, Guangyu Shi will examine the movement of proppant in the fracture and how the proppant is distributed in the fracture after injection stops. To understand the fate of proppant within fractures, a transparent physical model is being developed where proppant transport and slumping can be observed. The apparatus will allow observation of injection of proppant into the fracture and its layout within the fracture. This will enable a greater understanding of how the proppant maintains the opening of the fractures.



Results

So far, Guangyu has designed and built the apparatus to physically model single hydraulic fracturing and visualize it while it is being fractured by different stress states on the media. The placement of small-scale proppants will be examined in the apparatus. These results will be used to create a new model for transport of proppant within fractures.

Conclusions

- Apparatus for physically modelling hydraulic fracturing has been constructed and tested.
- The visualization system is capable of viewing the growth of the fracture in real time.
- Simple models for proppant transport are being explored.

Guangyu Shi acknowledges Schlumberger for the use of Petrel, Visage and Mangrove.

Improved and alternative energy recovery from petroleum reservoirs

Interactions of transition metal ions and petroleum in geological systems

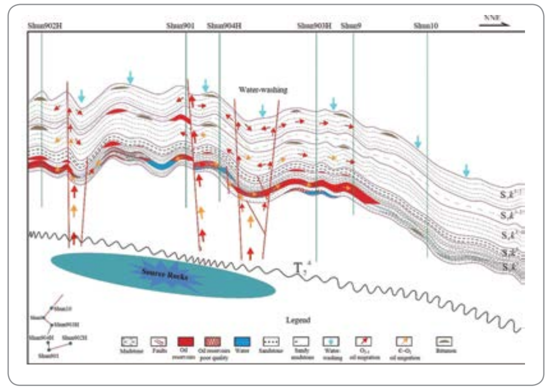
Qianru Wang
PhD student

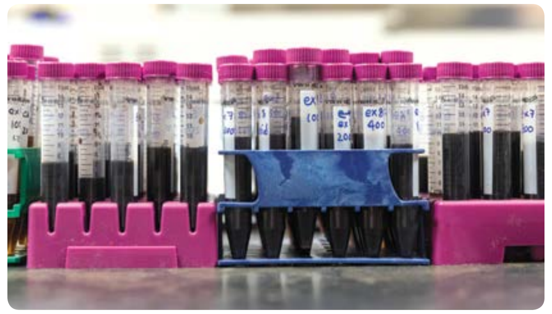
Introduction

As part of investigating the feasibility of using transition metals as energy carriers for energy recovery or for environmental cleanup, Qianru Wang is investigating the interaction of manganese and iron with crude oil and natural petroleum reservoirs to explore mechanisms and kinetics of reactions, using samples from China. The main challenge is that, in China especially, the samples from Tarim Basin, experienced multi-charging periods from different source rocks which influenced the oil composition. Hence, the source rock and charging time of each episode must be identified first by mineralogy, petrography and geochemistry analysis.

Results

Qianru has carried out a literature study of oxide alteration of hydrocarbons. She has also identified the hydrocarbon charging periods from different source rocks of all the samples from Tarim Basin. Oil composition of each charge episode has been analyzed. Multi-stage hydrocarbon accumulation mechanisms have been summarized in the study area. She will also examine natural settings in this and the Bohai and Ordos basins where metal ions may have interacted with reservoir oils.





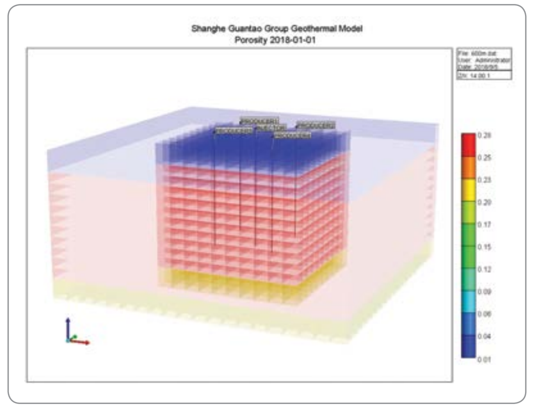
Conclusions

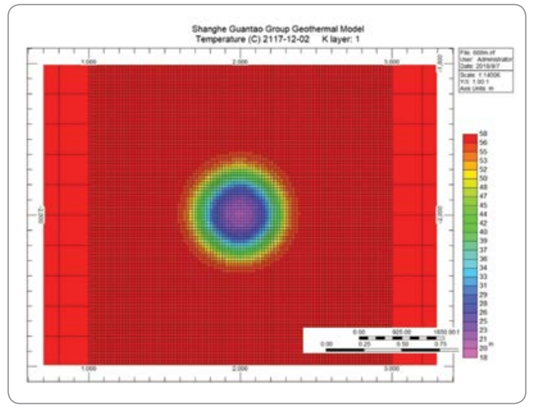
- Hydrocarbons in the Tarim Basin study area are from Cambrian-Lower Ordovician and Middle-Upper Ordovician source rocks.
- Hydrocarbons were charged in Late Caledonian (419.6-398.1 mega-annum), Late Hercynian (271.5-224.0 mega-annum) and during the Himalayan orogen (11.4-2.2 mega-annum).
- Oil composition of each episode changes significantly.

Qianru Wang acknowledges the support of China University of Geosciences, China University of Petroleum and China Petroleum & Chemical Corporation (SINOPEC).

Improved and alternative energy recovery from petroleum reservoirs

Qinwan Chong
PhD student





Introduction

As a part of her research, Qinwan Chong has constructed a detailed geological model and geothermal simulation model to understand the dynamics of geothermal processes with and without aquifers. She has evaluated the model with different well patterns and well spacing for injection and production of the heat transfer working fluid. Other process design parameters include the continuous or intermittent operation (e.g. operation during winter only or year-round). By comparing the outcome of different cases, the case with the best thermal breakthrough time has been selected. The biggest challenge has been how to design a reasonable and effective model that includes all of the key physics and most important geological features. Grid refinement in the area around the wells is required to more accurately solve the heat transfer problem surrounding the wells. Future work will include optimization of the process operating strategy and well placement to determine the most efficient geothermal process.

Results

Qinwan's results have demonstrated that the heat withdrawal from the system must be balanced with the natural heat provided to the geothermal system. In other words, some designs lead to rapid cooling of the geothermal system due to insufficient natural heat influx. Aquifers can provide a heat transfer fluid underground that tends to enable more natural heat influx. Continuous operation for 30 years can cool the geothermal system more than cases operated for four months each year for 100 years. Well spacing less than 600 meters leads to a more expensive operation with greater heat withdrawal from the geothermal system. Five well pads appear to show promise for over well configuration versus single injection and production wells.

Conclusions

- Balance between heat supply to geothermal system and heat withdrawal is critical to the process design.
- Non-continuous operation permits a longer operating period.
- A five-well pattern with more than 600 meter well spacing works better than a single injection-production configuration.
- Future work will explore effect of faults and geothermal gradient on process dynamics.

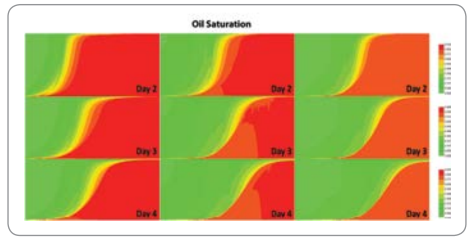
Improved and alternative energy recovery from petroleum reservoirs

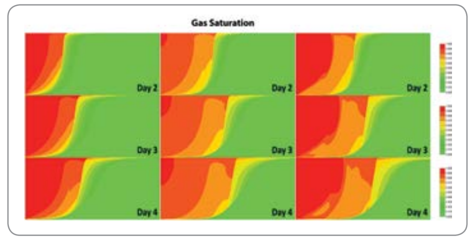
Mechanisms of flue gas EOR in heavy oil/oil sands system — small scale simulation study

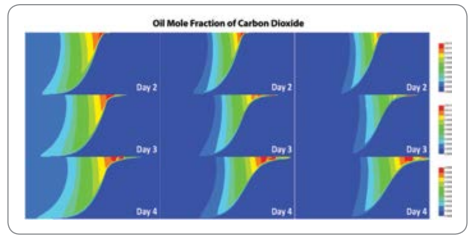
Ran Luo
PhD student

Introduction

Several field pilots have suggested positive results for a non-condensable gas co-injection with steam process for producing oil sands reservoirs with reduced emissions to oil ratio and improved energy efficiency. Ran Luo has conceived of an alternative process where heated flue gas is injected with no steam. The intent of this project is to examine the dynamics of heated flue gas at the edge of the depletion chamber by using a small-scale thermal reservoir simulation. The simulation model is a 50 centimeter by 10 centimeter 2D model and the grid dimensions are 1 millimeter in each direction. So far, Ran has examined the cases of 100 C, 200 C, and 300 C injections.







Results

The main results from Ran's research so far are that hot flue gas mobilizes oil and it drains under gravity and is produced from the system, and that the oil saturation gradient clearly is rich to lean, whereas the gas saturation gradient is complex at the edge of the chamber and the gradients occur over a 20 centimeter length-scale. By looking at profiles of saturation and composition, he has found that a quasi-steady state is established at the edge of the chamber. CO_2 builds at the edge of chamber but since diffusion is slow, limited CO_2 penetrates into oil. Thus, temperature dominates as the reason why the oil was mobilized.

Conclusions

Hot flue gas injection demonstrates that the process creates a depletion chamber with gravity drainage of mobilized oil. The process appears to be technically feasible.

The hotter the temperature of the flue gas, the faster the horizontal growth of the chamber and the more compressed are the profiles of saturations and compositions.

At hot temperatures, CO_2 is not acting as a solvent since its content in oil phase is low.

Ran Luo acknowledges Computer Modelling Group for the use of STARS™.

Improved and alternative energy recovery from petroleum reservoirs

Oil charge model under biodegradation in Athabasca oil sands area, Western Canada

Rui Chang
MSc student

Introduction

The intent of this project is to understand the biodegradation of oil as it fills a point bar deposit on a current reservoir in the Athabasca area. Through the biodegradation process, light oil is transformed into heavy oil and Co_2 and CH_4. Given the reaction system being used to model biodegradation, the results of the model will demonstrate how the chemical composition of the biodegraded oil varies spatially within the point bar as well as the spatial variability of the oil phase viscosity. The implication of the results is important for geochemical and geological exploration and for well placement for production operations.

Results

The main outcomes from Rui Chang's research so far have been an assessment of the 3D point bar model and construction of simpler 2D charge simulations to test the biodegradation reaction model. One key issue confronted by these models is that they are large and will have to run for up to several tens of millions of years.

Conclusions

Biodegradation depends on reservoir temperature, fresh oil charge rate and in-reservoir mixing rate.

For the Athabasca deposit, CO_2 gas content and steep oil compositional gradients indicate biodegradation activities.

Real reservoir simulation demonstrates the oil distribution after experiencing biodegradation.

Rui Chang acknowledges Computer Modelling Group for use of STARS™ and Schlumberger for use of Petrel and Eclipse.

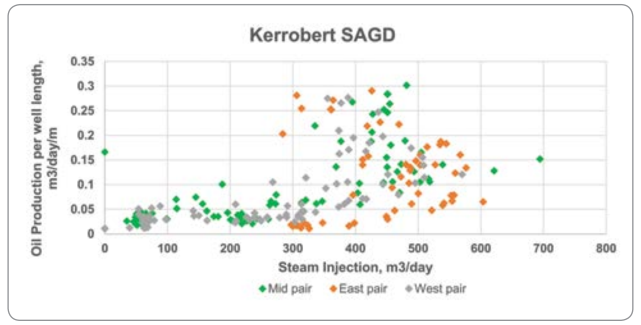
Improved and alternative energy recovery from petroleum reservoirs

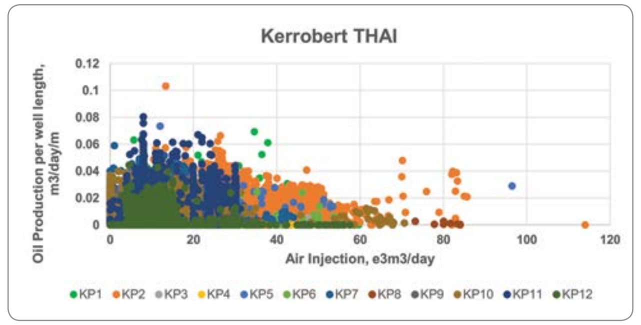
Analysis of Kerrobert THAI project

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, and from data mining and analytics, demonstrate the recovery mechanisms and strength 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.



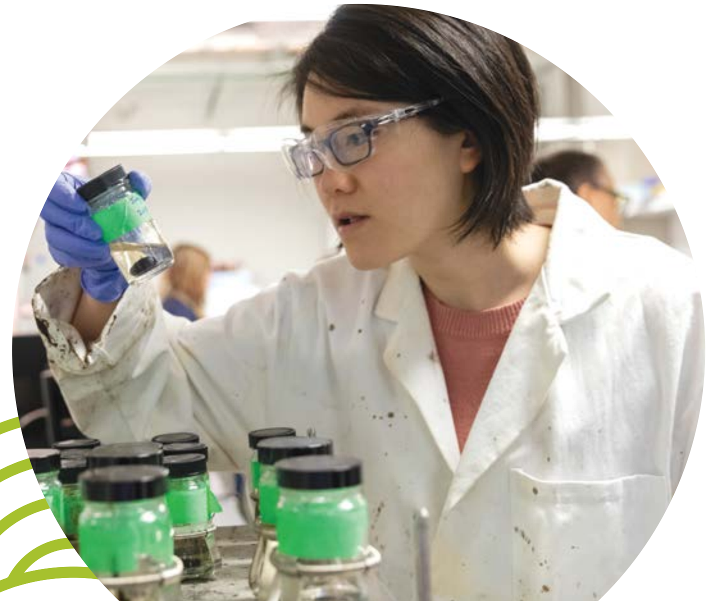


Results

In this research, Wei has developed diagnostics to determine causal relationships between injectants and production rates, gas composition and temperature rise within the reservoir. It has been found that there is no linear relationship between oil/water production and air injection. The produced gas volume increases linearly with air injection. Temperature and pressure data are examined but no clear relationship has been found between well temperature and air injection rates. The injector pressure has minimal change and producer pressure has no significant change by air injected. The produced gas composition and component ratios have also been evaluated and the low oxygen gas produced suggests that combustion (oxidation) reactions have taken place in the reservoir. Looking at the high production of carbon oxides, consumption of oxygen gas has indicated high temperature oxidation is more dominant than low temperature oxidation reaction. Comparison with steam-assisted gravity drainage (SAGD) project has yielded lower normalized oil production rate from THAI.

Conclusions

- The peak oil rate can be reached when air supply is at an intermediate value. Too little or excess air injection reduces oil production.
- High temperature oxidation is the dominant combustion reaction in this reservoir during air injection.
- The THAI process has relatively shorter drainage front than that of SAGD, thus yielding lower normalized oil production rate than that of SAGD.



Wei Wei acknowledges Proton Technologies for permission to use their data, and Mitacs for the financial support through a Mitacs-Accelerate Graduate Research Internship Program.

Improved and alternative energy recovery from petroleum reservoirs

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

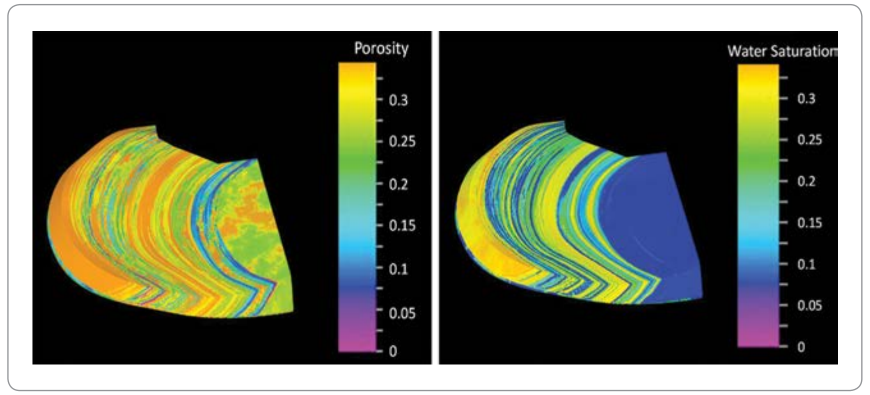
Yi Su
Postdoctoral Fellow

Introduction

The intent of the project is to find new operating strategies to reduce CO_2 emissions in unconventional oil recovery operations. In the context of geological complexity, the following three objects need to be considered: (1) oil recovery (2) steam reduction and (3) operation costs. The study will determine how geology impacts recovery method by examining the energy efficiency and the emissions per unit of oil produced. The finding will provide guidelines on how to choose the best recovery methods under geological complexity leading to economic operations with low environmental effects.

Results

The main outcomes of Dr. Yi Su's research so far are a comparison between steam-assisted gravity drainage (SAGD), expanding solvent steam-assisted gravity drainage (ES-SAGD) and pure solvent injection in a complex oil sands point bar deposit. The results have shown that heterogeneity of the formation affects the performance of the recovery process and that solvent can lead to improved performance with respect to energy efficiency and environmental impact but that the economics can suffer due to solvent retained in the reservoir. The retained solvent can be lost both under and over shale layers within the point bar.



Conclusions

- Solvent-aided steam injection can improve energy efficiency and environmental impact performance.
- Solvent recovery factor is very important for thermal solvent processes since it strongly affects economics.
- Complex geological structure could lead to low solvent recovery — heat moves through shale layers but solvent does not.
- Warm solvent process is very sensitive to reservoir quality with respect to solvent retained in the reservoir.

Dr. Yi Su, PhD, acknowledges Computer Modelling Group for use of STARS™ and Schlumberger for use of Petrel and Eclipse.

Improved and alternative energy recovery from heavy oil reservoirs

Yong Ma
Postdoctoral Fellow

Introduction

This project is part of the study of the interaction of metal oxides and crude oils mediated through microbial activity in petroleum and natural gas reservoirs. Dr. Yong Ma, PhD, will sample core and cuttings, oil and gas material from reservoir and source rock sections in China from Bohai Bay Basin, Ordos Basin and Sichuan Basin, and analyze them using both inorganic and organic geochemical methods. Comparison of reference sample sets with oxidized and reduced metal species and crude oils will be made to allow him to identify, through molecular analysis of appropriate oil and gas samples, the nature and processes of anaerobic biodegradation taking place. In this study, he will also examine direct, abiotic, oxide hydrocarbon interactions.

Results

Yong has performed sampling of reservoir, source rock and produced oil samples from Shengli oilfield. He took part in a research team visit to Dongying in May. Separately, he collected the red beds and "bleached" sandstones from the Jurassic and Cretaceous section in the Ordos Basin in China, and has started to run the pyrolysis and thin section experiments. Examining hydrocarbon interactions with minerals and organic matter, he has also conducted long-term canister desorption of organic-rich shales from the Sichuan Basin to study the chemical and isotopic compositions variations of released gases. Both CO_2/CH_4 and ethane (C_2H_6)/CH_4 ratios of the released gas increase with extended desorption, while the C_2H_6/CH_4 ratio decreases after the peak. The chemical compositional variations seen during desorption are caused by the difference of adsorption capacity and molecular size of CH_4, C_2H_6 and CO_2. Delta thirteen C ($\delta^{13}C$) values of desorbed methane and ethane increases sharply with increasing volumes of gas released at reservoir temperature. Desorbed gas composition after five hours of desorption approximately represents the carbon isotopic composition of the *in situ* gases.

Conclusions

- Sampling programs from two Chinese basins are complete and key experiments are underway.
- Naturally bleached iron oxide containing sediments are being studied.
- Gases released from canister desorption at different temperatures have been analyzed to study hydrocarbon interactions with mineral phases and organic matter.

Dr. Yong Ma, PhD, acknowledges the support of Mitacs.

BEIJING RESEARCH COLLABORATION

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 framework 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

Bukola Olusola is working with drill cuttings of Mexican carbonates. His work is in progress and he is conducting laboratory work for determining porosities and permeabilities from those drill cuttings. In the future, he will attempt to integrate these results with the correlation developed by his research team for estimating the Biot coefficient.

Results

As his experiments are in progress, Bukola's outcomes are still under evaluation. But given his past extensive experience evaluating drill cuttings collected in vertical and horizontal wells he anticipates that his results will prove valuable for integration with the Biot correlation coefficient developed by his research team.

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

Qi Li
PhD student

Introduction

Qi Li participates in the development part of a correlation for estimating Biot coefficient. This is important as Biot coefficient plays an important role in solving many practical petroleum engineering problems, including for example, design of hydraulic fracturing jobs. Biot coefficient is closely related to compressibility, determination of which is the ultimate objective of this research. The correlation has application in conventional and unconventional petroleum reservoirs, and it is being developed in such a way that it will also have application for estimating Biot coefficient in the case of unconsolidated petroleum reservoirs and oil sands.

Results

The main outcome of Qi's research has been the development of a new practical correlation for estimating Biot coefficient. He has performed a detailed literature survey and has determined that his idea for estimating Biot correlation has not been considered previously in the literature. Thus, he started working on the idea and has come out with an original correlation where Biot coefficient is determined as a function of permeability, porosity and pore throat aperture.

Conclusions

Development of an original correlation (still being refined) that integrates Biot coefficient, permeability, porosity, pore throat aperture and compressibility.

The originality and uniqueness of the correlation is that it has application in carbonates, sandstones, shales, marble, granite, unconsolidated sand and oil sands.

Qi Li acknowledges PEMEX and CONACYT.

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

Jiri Hostas
Postdoctoral Fellow

Introduction

It is of high strategic relevance and economic benefit to reduce the need for diluent in bitumen and heavy oils to reach pipeline transportability. The catalytic system for upgrading of extra-heavy oils recently uncovered in the lab represents one way to tackle this challenge. Dr. Jiri Hostas, PhD, focuses on understanding the atomistic mechanisms of chemical reactions in complex environments involved in heavy oil upgrading. Molybdenum sulphide (MoS_2) is being developed as a hydrogenation and coke-prevention catalyst and Jiri is interested in how MoS_2 nanoparticles are interacting with an asphaltene and with silica and calcium carbonate rock.

Results

As a part of his research, Jiri has used density functional theory (DFT) with deMon2k software to explore the interactions between and among a 48-atom model for a MoS_2 nanoparticle, a 61-atom quinolin-65 model for asphaltenes and models for calcium carbonate and silica containing about 50 atoms. He has obtained preliminary results for binding energies for a single local minimum-energy configuration for each case. Catalyst binds strongly to the rock with silicate being somewhat stronger than carbonate. The catalyst also binds strongly to the asphaltene. Interactions between the asphaltene and the rock are considerably weaker. Currently, the project is being extended to DFT-BOMD and Minima Hopping methods for starting-structure determination, using the local density approximation and severely-pruned auxiliary function sets as a fast methodology for exploring the potential-energy surface to find local minima.

Conclusions

Jiri has provided additional confirmation of an indirect experimental evidence that the catalyst is being strongly bound to both asphaltene and the rock. On the contrary, asphaltene does not demonstrate strong affinity to the rock.

This is important for understanding of catalyst transporting processes *in situ* and further catalyst improvements.

Dr. Jiri Hostas, PhD, acknowledges SENER and CONACYT of Mexico for support of this work and Compute Canada and WestGrid for the provision of computational resources.

Development of an oxy-cracking process scheme for demineralizing (metals removal) and converting petroleum coke into commodity chemicals

Abdallah Darweesh Manasrah
Postdoctoral Fellow

Introduction

Dr. Abdallah Darweesh Manasrah, PhD, focuses on researching oxy-cracking as a new innovative technology for creating economic value from any residual feedstocks like petcoke, oil sands bitumen, residue streams and mine-reject asphaltenes by converting them into valuable products such as humic acids, clean fuel and metals recovery. This is novel and is a combination of oxidation and cracking (i.e. oxy-cracking) processes in an aqueous alkaline media at moderate temperatures (approx. 170 C) and pressures (300-500 psi) with relatively low proportions of water. This process is explored to enhance settling in process-affected water of oil sands.

Results

Abdallah investigates the effect of oxy-cracking temperature on the hydrocarbon solubilisation and settling. The oxy-cracked products have been characterized using Fourier-transform infrared spectroscopy (FTIR) and compared with commercial humic acid. Also, the metal and sulfur contents of the oxy-cracked products have been analyzed. The results have suggested that the proposed process could be employed for petcoke demineralization and desulfurization and enhanced settling in tailing. This technique provides promising results for the enhancement of fine particle settling without the emission of CO_2; i.e. it is environment-friendly as well as cost-effective.

Conclusions

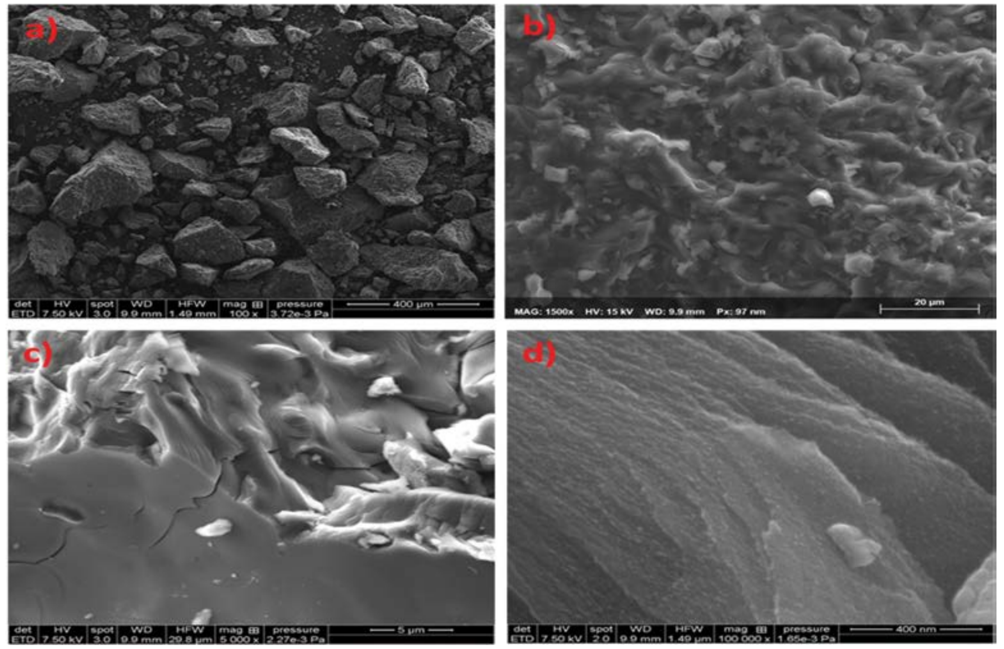
The key benefit of this technology is not only the high efficiency, conversion and selectivity for desired products but also zero direct CO_2 emission.

Moreover, this technology could be applied for demineralization and desulfurization of residue streams.

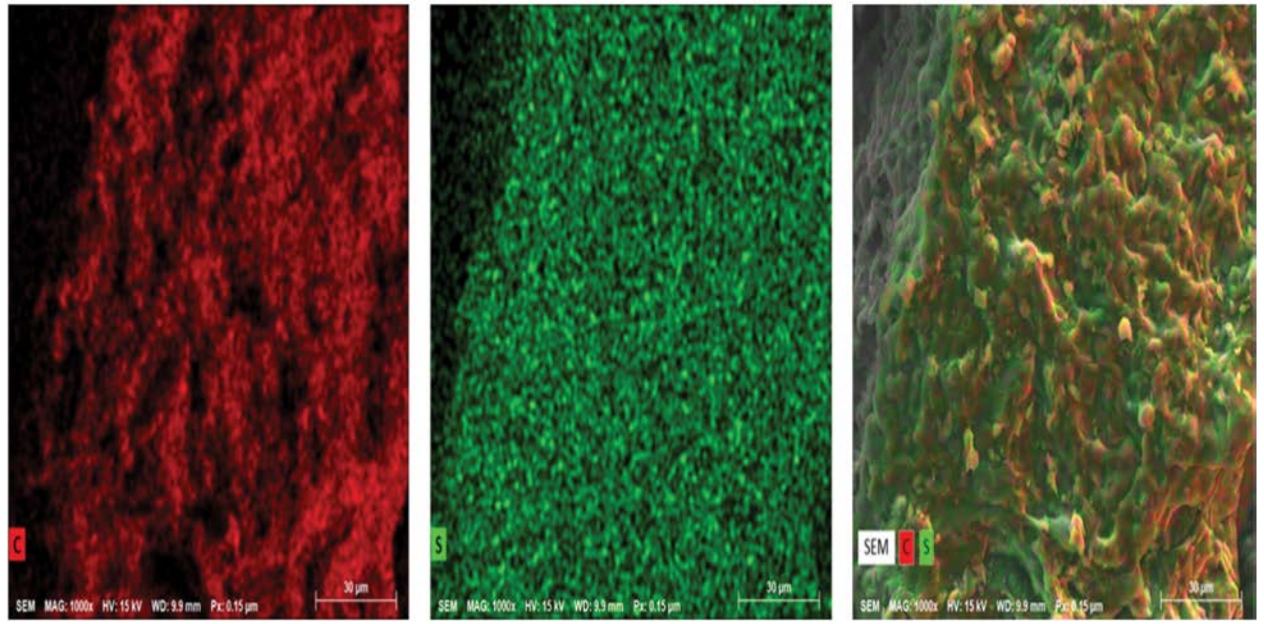
The technology promises to provide an alternative, efficient, environment-friendly and cost-effective technology to convert residual feedstocks into humic acids.

Dr. Abdallah Darweesh Manasrah, PhD, acknowledges the Mexican industrial partner for financial support.

Absence of porosity in petroleum cokes



Presence of carbon and sulfur on petroleum coke surface (EDAX analysis)



KNOWLEDGE NETWORK: SOLUTIONS FOR MATURE OIL FIELDS AND UNCONVENTIONAL FIELDS

Hossein Hejazi, Sudarshan (Raj) Mehta, Robert (Gordon) Moore,
Jerry Jensen, Thomas Oldenburg, Per K. Pedersen, 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 inter-well 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 re-evaluation 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.

Optimizing oil extraction from mature fields through the analysis of fluid heterogeneities: 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 works 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 (FTICR-MS). 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.

Using nanofluids and micro-reservoirs to enhance oil recovery from mature fields in Mexico: In most oil fields, more than two-thirds of 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.

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.

Optimizing oil extraction from mature fields through the analysis of fluid heterogeneities

Aprami Jaggi
Postdoctoral Fellow

Introduction

Dr. Aprami Jaggi, PhD, aims to develop a comprehensive methodology to define reservoir compartmentalization models in mature oil fields, using cutting edge geochemical techniques, geological information and reservoir engineering, to increase the petroleum production. Fresh oil samples need to be collected for the study. The oils from the original study area are too viscous to produce and collect, so a new study area needs to be determined and sampling arrangements made. Shipping and customs challenges have further delayed the progress of the project.

Results

Aprami has carried out a literature review of the study areas. She received seven extra-heavy oil samples and performed comprehensive geochemical analysis using bulk measurements, gas chromatography mass spectrometry and ultrahigh resolution mass spectrometry techniques, namely Fourier-transform ion cyclotron resonance mass spectrometry.

Conclusions

- The geochemical characterization reveals multiple charge histories of some of the oils.
- The seven oil samples have been distinguished to fall into three families.

Advanced characterization and innovative solutions for the recovery of heavy oil in mature fields

Dario Harazim
Postdoctoral Associate

Introduction

Mexico possesses substantial unconventional hydrocarbon reserves in the southeastern part of the country. However, the production of these oil reserves is challenging due to the high viscosity of the oil and the challenging architecture of the oil reservoir itself. Dr. Dario Harazim, PhD, aims to transfer expertise in the area of reservoir and fluid characterization for heavy oil reservoirs to the Mexican partners. The University of Calgary is planning to convey knowledge about workflows for Alberta-developed reservoir characterization to the Mexican academic partners. The University of Calgary is ideally positioned in this collaboration given its role as the global player in research on heavy oil (bitumen) production technology and forecasting. The opening of the Mexican hydrocarbon sector in 2013 also provides a unique opportunity for University of Calgary researchers to expand their research network and deliver solutions to other heavy oil deposits worldwide.

Results

Dario has completed the first iteration of a reservoir heterogeneity model for Samaria Field (Tabasco, Mexico). This reservoir model has been integrated into a static petroleum reservoir model built by the ITPE in Merida, Yucatan. This first model is now complete and about to be handed over to the IMP in Mexico City, for first flow simulation experiments. Understanding the reservoir connectivity of Samaria Field has proven to be more challenging than initially expected given the low seismic resolution and the relatively wide well-spacing at Samaria. One of the main objectives for the upcoming phase II is the re-evaluation of the standing reservoir stratigraphy and upscaling of observed reservoir heterogeneities. A second and possibly third iteration of the Samaria reservoir model is being planned for 2019 and 2020.

Conclusions

Dario and his research team have broken ground in an area that opened to international researchers only five years ago.

Samaria Field is internally highly compartmentalized and structurally complex.

The standing seismic volume for Samaria Field does not sufficiently resolve pool boundaries.

A new reservoir connectivity workflow, specifically for Samaria Field is being developed by Dario, Prof. Per K. Pedersen and Prof. Thomas Oldenburg that will address the standing reservoir connectivity challenges.

Dr. Dario Harazim, PhD, acknowledges the Mexican partners at ITP in Mexico City and ITPE in Merida, Yucatan for their timely delivery of research samples and internal government reports. Dr. Harazim also acknowledges CABS for their support with software setup and assistance with reservoir modelling workflows.

Advanced characterization and innovative solutions for the recovery of heavy oil in mature fields

Jagos Radovic
Postdoctoral Associate

Introduction

Dr. Jagos Radovic, PhD, aims to build an integrated geological reservoir characterization and a petroleum fluids characterization to optimize the development of a Mexican mature field by using enhanced oil recovery solutions based on steam-solvent-surfactant injection. He is investigating vertical connectivity of reservoir compartments by studying fluid heterogeneities. Timing schedules are challenging as Jagos depends on fresh cuttings collected during well drilling and shipping of the samples to Calgary.

Results

After sampling, sample selection, and customs challenges Jagos has finally received 60 samples from the first well drilling event. He has prepared the samples for petroleum geochemical analysis using liquid extraction techniques and has established an oil and water saturation reservoir profile. Saturated and aromatic hydrocarbons have been analyzed using a gas chromatograph coupled to a mass spectrometer. The interpretation of the data is currently under investigation.

Conclusions

Fresh drilled well cutting samples have been received from one well.

Geochemical investigations are ongoing and yet to arrive at a conclusion.

MEXICO RESEARCH COLLABORATION

PUBLICATIONS

Publications in peer-reviewed journals

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SUPPORTING ORGANIZATIONS

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- Suncor Energy Inc.
- The China National Petroleum Corporation (CNPC)

GLOSSARY OF ACRONYMS

AE	Anion exchange
AEM	Anion exchange membrane
AFM	Atomic force microscopy
Al_2O_3	Aluminium oxide
AQP	Catalytic aqua processing
AVECS	Alternative vectors for carbon storage
BHP	Bottom hole pressure
C-1	One carbon
C_2H_2	Acetylene
C_2H_6	Ethane
CaMI	Containment and Monitoring Institute
CCS	Carbon capture and storage
CFREF	Canada First Research Excellence Fund
CH_4	Methane
CLS	Canadian Light Source
CNC	Cellulose nanocrystals
CNF	Cellulose nanofibril
CO	Carbon monoxide
CO_2	Carbon dioxide
CO_2RR	Electroreduction of CO_2
CO_3^{2-}	Carbonate ion
Cr	Chromium
cryo-SEM	Cryo-scanning electron microscopy
cryo-TEM	Cryo-transmission electron microscopy
CuBDC	Copper benzenedicarboxylate
$\delta^{13}C$	Delta thirteen C
DC	Double couple
DCA	Decline curve analysis
DCSG	Direct contact steam generators
DFT	Density functional theory
DLVO	Derjaguin, Landau, Verwey and Overbeek theory
DPDK	Dual porosity-dual permeability
EA	Elemental analysis
ECS	Energy conversion and storage
EOR	Enhanced oil recovery
ERT	Electrical resistivity tomographies
ES-SAGD	Expanding solvent steam-assisted gravity drainage
FC	Fuel cell
Fe_2O_3	Ferric oxide
FPG	Free phase gas

FRS	Field Research Station
FTICR-MS	Fourier-transform ion cyclotron resonance mass spectrometry
FTIR	Fourier-transform infrared spectroscopy
FWI	Full-waveform inversion
GHG	Greenhouse gas
GM	Gas migration
GO	Graphene oxide
GRI	Global Research Initiative in Sustainable Low Carbon Unconventional Resources
HaP	Hydroxyapatite
HQP	Highly qualified personnel
H-PML	Hybrid-perfectly matched layer
HPHT	High pressure, high temperature
H-SOFC	Proton conducting solid oxide fuel cells
HTI	Horizontal transverse isotropic
ICPMS	Inductively coupled plasma mass spectrometry
IFT	Interfacial tension
IPN	Interpenetrating network
ISGP	Impedance spectroscopy genetic programming
L-BFGS	Limited-memory Broyden-Fletcher-Goldfarb-Shanno
LCA	Life cycle assessment
LCST	Lower critical solution temperature
LRS	Liquid-rich shale
LSCM	Laser scanning confocal microscopy
mA/cm^2	Milliamperes per square centimeter
MFC	Microbial fuel cell
MFHW	Multi-fractured horizontal wells
$MgCl_2$	Magnesium chloride
MIEC	Mixed ionic and electronic conducting cathode
MOF	Metal-organic framework
MoS_2	Molybdenum disulfide
MS	Mass spectrometry
Mw	Moment magnitude scale
NaCl	Sodium chloride
NCS	Nanoporous scaffold
NFR	Naturally fractured reservoir
NHC	N-heterocyclic carbenes
Ni	Nickel
NMR	Nuclear magnetic resonance
NOx	Nitrogen oxides
NP	Nanoparticle
NPV	Net present value
NR	Neutron reflectrometry
NS	Nanosheets
OPV	Organic photovoltaics
ORR	Oxygen reduction reaction

PAM	Polyacrylamide
pCO_2	Partial pressure of carbon dioxide
PEDOT: PSS	Poly (3, 4-ethylenedioxythiophene): poly(styrenesulfonic acid)
PFM	Photonic force microscopy
PLD	Pulsed laser deposition
PNIPAm	Poly(N-isopropylacrylamide)
Pt	Platinum
PTDG	Total dissolved gas pressure
PV	Photovoltaic
PVT	Pressure volume temperature
Q-RTM	Viscoacoustic reverse time migration
ReaxFF	Reactive molecular dynamics method
RTA	Rate transient analysis
RTM	Reverse time migration
SAC	Single atom catalyst
SAGD	Steam-assisted gravity drainage
SCVF	Surface casing vent flows
SDS	Sodium dodecyl sulfate
SEM	Scanning electron microscope
SF	Safety factor
SH	Shear
S_{Hmax}	Maximum horizontal stress
SiO_2	Silicon dioxide
SMMR	Surface-mimetic micro-reservoir
SOEC	Solid oxide electrolysis cell
SOFC	Solid oxide fuel cell
SOx	Sulphur oxides
SRV	Stimulated reservoir volume
SWD	Seismic-while-drilling
TTACT	University of Calgary Technology Assessment and Coordination Team
TAPPy	1,3,5-triazapentadienyl-2,4-bis(2-pyridyl)
TEM	Transmission electron microscopy
THAI	Toe-to-heel air injection
TOC	Total organic carbon
ToC2ME	Tony Creek dual microseismic experiment
TPP	Tetra(phenyl)porphyrins
TThP	Tetra(thiophenyl)porphyrins
TTI	Tilted transverse isotropic
TVD	True vertical depth
UAV	Unmanned aerial vehicle
UHR	Unconventional hydrocarbon resources
VTI	Vertical transverse isotropic
WAG	Water alternating gas
XRD	X-ray diffraction
YSZ	Yttria-stabilized zirconia

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