



ALBERTA INGENUITY CENTRE FOR IN SITU ENERGY

Summer Newsletter 2009

The Alberta Ingenuity Centre is set to transform the oil sands industry. We have brought together many of the world's leading innovative scientists, industry and other partners to develop more efficient, cost-effective and environmentally sustainable processes and practices for in situ recovery and upgrading of Alberta's oil sands resource- all with extremely low environmental impacts.

This issue of the AICISE newsletter contains updates on the CCIT Expansion project, introduces a bold new educational outreach partnership with CMASTE, spotlights new members and provides a brief description of several recent publications surrounding on-going research.

The Centre is proud to announce the launch of our new website, which can be found at <http://www.aicise.ca>. Come visit us to find out more about the Centre's exciting new research!

CCIT Expansion Project Update

AICISE has recently received the **Bruker 12 T Fourier Transform Ion Cyclotron Mass Spectrometer**, which will allow a much more comprehensive analysis of most complex organic mixtures such as petroleum. The high-field FT-ICR-MS will improve the understanding and characterization of hydrocarbon conversion during *in situ* upgrading processes, which includes comprehensive monitoring of the structural modifications of bitumen macromolecules. It will result in an increasing knowledge of chemical reactivity patterns and the physical/chemical properties of the constituent molecules. This understanding is essential to support the recovery of bitumen confined in *in situ* upgrading, and to selectively enhance the bitumen properties such as viscosity and acidity.



The Bruker 12 T FT-ICR-MS would provide, for the first time, an unparalleled window into the complexity of petroleum and will make the Centre outstanding in petroleum research in the world.

Learn more about the Bruker 12 T FT-ICR-MS at http://aicise.ca/what%27s_new/CCIT.

May 6th, 2009 Meetings

The AICISE **Management Advisory Board (MAB)** met on May 6, 2009 at the University of Calgary. The MAB is AICISE's primary governing body and forms the apex of the governance structure.

Dr. Pereira-Almao along with Dr. Maini, select research associates and partner representatives came together for a successful **Peer Assist** meeting to discuss the Centre's research. Special invitee Deborah Sword facilitated.

Meet New Faces at AICISE



Kharim Ghesmat
New Post Doc
Reservoir Simulation



Zahra Fatouraei
Research Technician
In Situ Combustion



Hector Guzman
Intern Student
Catalysis



Andrew Carss
Intern Student
Catalysis

Outreach with the Centre for Mathematics, Science and Technology Education (CMASTE)

The Centre is proud to announce a partnership with [CMASTE](#), an education research centre at the University of Alberta that focuses on curriculum development for students grades K-12. In July of this year, two high school teachers (Sarah Lazowski and Verna McKinnon) will join with researchers at the Centre to develop lesson plans that reflect our current research and combine them with the Alberta curriculum.

CMASTE's unique integrated R&D approach to education enhancement makes them well matched to Alberta Ingenuity Centres and allows students to learn more about vital resources in their area and the future of science and technology.

Industrial Catalysts & Catalytic Reactors Course

On April 28th-30th, students were able to attend a course presented by Dr. Jacques Bousquet which focused on the importance of catalytic material and the reactor in the process of catalysis. Topics included "Catalysis for automotive depollution", "Process to convert natural gas into liquid fuels", "Catalysis energy and CO₂" and more.

Dr. Bousquet received his PhD, MSc, and BSc from L'Ecole Supérieur in Lyon, France and has worked for ELF Atochem and ELF Aquitaine (which later became TOTAL). He has
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submitted more than thirty patents and forty publications as well as numerous presentations. He is currently the general manager of the Federation Gay-Lussac (FGL) (which coordinates all the 18 chemical engineering schools in France) and Vice President of the "industrial chemistry division" of the Société Française de Chimie.

IV Annual Meeting of CBUHyP

Last month, the IV Annual Meeting of the Catalysts for Bitumen Upgrading and Hydrogen Production (CBUHyP) was held in the Rosza Centre at the University of Calgary. Beginning on May 4, Dr. Pedro Pereira-Almao (lead researcher) emphasized the main activities to be developed in the near future. External attendees included industrial sponsors such as: Shell, ConocoPhillips, and Nexen as well as other invited researchers.

The meeting was divided into Internal Projects and AICISE related projects. The AICISE projects, which comprise the main research efforts of the CBUHyP

group, included 22 presentations for exposing the research accomplishm



ents in such diverse areas as: Catalysts and Adsorption for In-Situ Upgrading; Design and Synthesis of Catalysts and Novel Materials; Engineering for Simulation and Scaling-Up; as well as Characterization of Bitumen and Products.

Potential for Hydrogen Generation during In Situ Combustion of Bitumen

Description

The volume of heavy oil and bitumen in Alberta, Canada is similar to that of the conventional crude oil in the Middle East. A large fraction of Alberta's bitumen is upgraded in surface upgraders to synthetic crude oil which plays a significant role on the energy supply of Canada.

Upgrading bitumen requires hydrogen; often this hydrogen is sourced from natural gas which undergoes steam methane reforming together with the water-gas shift reaction. The potential for in situ generation of hydrogen by gasification of bitumen reservoirs offers an attractive alternative which can also have both economic and environmental benefits.

Application

Applications of this research are in hydrogen production for surface upgrading, in situ upgrading, and as a feedstock for ammonia and other chemicals. In situ gasification provides an attractive means for generating hydrogen with potential for sequestering carbon oxides directly in the reservoir so emissions to atmosphere are reduced.

Results

This study evaluates the effect of operating parameters such as temperature and pressure on the amount of hydrogen generated during in situ combustion. Combustion of Athabasca

bitumen incorporating thermal cracking, oxidation, and hydrogen generation and consumption reactions have been simulated.

For bitumen, hydrogen generation occurs under the general reaction:



and the water-gas shift reaction:



together with coke gasification, and hydrogen consumption by methanation and hydrogen combustion reactions.

The results indicate ranges of temperature and pressure where bitumen combustion yields optimal hydrogen production.

Significance

The current research emphasizes the conditions at which hydrogen production can be maximized from in situ combustion of bitumen. This technology provides a potentially clean method to produce fuel and feedstock material from bitumen, a relatively "dirty" fuel and feedstock oil.

View this publication at
<http://aicise.ca/node/382>.

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Estimation of Kinetic Constants for in situ Ultra-Dispersed Catalytic Upgrading of Bitumen on a Batch Reactor

Description

In situ catalytic upgrading of heavy oil and bitumen has been proposed and tested in laboratory-scale experiments and experimental indications from these laboratory-scale tests show potential for in situ upgrading of bitumen and heavy oil using an ultra-dispersed catalyst. This novel technique may play an important role in the development of the huge resources of heavy oil and bitumen in Alberta. In this paper, we present reaction constants estimation for ultra-dispersed catalytic upgrading experiments conducted in a batch reactor. The Monte Carlo simulation technique is used to find the most appropriate reaction constants. Combination of an analytical batch reactor model and the Monte Carlo simulation technique allow rapid generation of a large number of upgrading experiment realizations. Large numbers of upgrading experiment realizations are used to estimate the kinetic constants at different temperatures. Comparisons of analytical modeling results with the experimental measurements of the upgrading experiments at different temperatures are in close agreement. Accurate parameters estimation of the new upgrading process is essential in order to correctly interpret experimental measurements, leading to a better understanding and design of industrial-scale processes.

Related Publications

H. Hassanzadeh; C. Galarraga; J. Abedi; Z. (John) Chen; P. Pereira Almas. Modelling of Bitumen Ultradispersed Catalytic Upgrading Experiments in a Batch Reactor. Conference paper presented at the Canadian International Petroleum Conference (CIPC), May 16, 2009

View this publication at
<http://aicise.ca/node/352>.

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