McGill

POLYTECHNIQUE MONTRÉAL
LE GÉNIE EN PREMIÈRE CLASSE

Departments of Chemical Engineering

Chemical Engineering Research Day

Tuesday, March 15 , 2016

8:30 AM – 6:00 PM

McGill, New Residence Hall

This event is sponsored by:

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PYROGENESIS

General Program

8:30 Arrival/ Registration

9:00 Welcome message (McGill New Residence Hall)

9:05 Plenary lecture: Dr. Jocelyn Doucet , CEO Pyrowave

10:00 Coffee break

10:15 Presentations (Parallel sessions)

12:15 Lunch break (Main Hall)

13:15 Plenary lecture: Prof. Peter Englezos, Chair and Professor, Department of Chemical Engineering, University of British Columbia

14:15 Presentations (Parallel sessions)

15:20 Coffee break

15:35 Presentations (Parallel sessions)

16:40 Wine & Cheese + poster session (Main Hall)

Plenary lectures will be in the McGill New Residence Hall

Ballrooms A & B

New Residence Hall

McGill University

3625 Avenue du Parc

Chairs:

McGill University: Profs. Christopher Moraes and Corinne Hoesli

Polytechnique Montréal: Profs. Jason R. Tavares and Nick Virgilio

Seminar Sessions

Session 1 -Track A: Ballroom A

Start*	Name	Supervisors	Title
9:05	**Plenary lecture**		
	Dr. Jocelyn Doucet, P. Eng., Ph. D CEO Pyrowave		• Improving resource efficiency to address climate change by observing Nature
10:00	**Coffee break**		
10:15	Davide Carnevali	G.S. Patience	• Conversion of glucose to C-6 carboxylic acids
10:28	Meghan Marshall	V. Yargeau	• Validation of LuminoTox as a tool to monitor wastewater toxicity
10:41	Hassana Elzein	R. Samson	• Development of an optimized-consequential life cycle assessment methodology and its application to the electricity generation sector
10:54	Mahmoudreza Aghighi	J. Gostick	• Simulation of a Full Fuel Cell Membrane Electrode Assembly Using Pore Network Modeling
11:07	Nury Ardila,	M.C. Heuzey and A. Ajji	• Chitosan/bacterial cellulose nanofibrous structures by coaxial electrospinning for wound dressing applications (with N. Medina, M. Arkoun and C.J. Panchal)
11:20	Remi Laraque	S. Coulombe and S. Omanovic	• MWCNT/Pt composite electrode with reduced Pt loading for hydrogen evolution reaction
11:33	Faezeh Sabri	N. Virgilio, J. R. Tavares, and L. Fradette	• Design and Characterization of Surface Modified microparticles with stimuli-sensitive and reversible aggregation/disaggregation behavior
11:46	Zeina Baalbaki	V. Yargeau	• Measurement and prediction of removal of contaminants of emerging concern during wastewater treatment
11:59	Mohammad Jaber Darabi Mahboub	G.S. Patience	• Gas phase oxidation of 2-methyl 1,3 propanediol to methacrylic acid over heteropolyacid catalysts
12:15	**Lunch break (Main Hall)**		
13:15	**Plenary lecture**		
	Prof. Peter Englezos Chair and Professor, Department of Chemical Engineering, University of British Columbia		Science and engineering of clathrate (gas) hydrates and applications in CO_2 capture and storage and safe hydrocarbon transportation

*Talks are 13 minutes in duration for graduate students including 3 minutes questions period.

Thank you for attending

Seminar Sessions

Session 2 -Track A: Ballroom A

Start*	Name	Supervisors	Title
14:15	Mounia Arkoun	M.C. Heuzey and A. Ajji	• In vitro and in situ study of antibacterial properties of electrospun chitosan-based nanofibers.
14:28	Agil Azimzada	N. Tufenkji and K.J. Wilkinson	• Characterization of Silver Nanoparticles in Wastewaters and Understanding their Interaction with the Green Alga, Chlamydomonas reinhardtii
14:41	Donya Farhanian	J.R. Tavares and G. De Crescenzo	• Preparation and Characterization of Thin Polymer-like Coatings on Silicon via Photo-Initiated Chemical Vapor Deposition (PICVD)
14:54	JingSi Jiang	J. Kopyscinski	• Development of Catalyst Coating for an Optically Accessible Plate Reactor
15:07	Ivan Viveros Santos	L. Deschênes, C. Bulle	• Accounting for geographic variability and speciation in the terrestrial ecotoxicity of copper. Case study of wine consumption in Quebec, Canada
15:20			**Coffee break**

Session 3-Track A: Ballroom A

Start*	Name	Supervisors	Title
15:35	Mahmoud Rammal	S. Omanovic	• Electrochemical reduction of CO_2 to low-molecular-weight organic molecules
15:48	Zhenni Ma	G.S. Patience	• Catalytic partial oxidation of methane over Pt/Rh catalysts supported on FeCralloy fibre
16:01	Charles Bruel	G.S. Patience and S. Coulombe	• CO_2 reduction on Pt-YSZ solid-oxide electrolysis cell
16:14	Alison Fraser	J. Gostick and J. Barralet	• Graphene oxide-metal oxide composite catalyst support for alkaline fuel cells
16:27	Clara Tromson	L. Deschênes and C. Bulle	• Enhancing the terrestrial ecotoxicological effect modeling of metals in life cycle impact assessment
16:40	**Poster session / Wine and cheese (Main Hall)**		

*Talks are 13 minutes in duration for graduate students including 3 minutes questions period.

Thank you for attending

Seminar Session

Session 1-Track B: Ballroom B

Start*	Name	Supervisors	Title
10:15	Larissa Jorge	S. Coulombe and P.-L. Girard-Lauriault	• Effect of Heat and Water on the Stability of Plasma Polymers for Functionalization of Carbon Nanotubes
10:28	Adya Karthikeyan	S. Coulombe, and A.-M. Kietzig	• Surface wetting and surface tension of stable and unstable carbon nanotube nanofluids
10:41	Nooshin Saadatkhah	G.S. Patience	• Catalyst preparation for fluidized bed reactors by spray drying
10:54	Jean-Sébastien Renault-Crispo	P. Servio and S. Coulombe	• Kinetics of carbon dioxide gas hydrates with the combination of tetra-n-butylammonium bromide and functionalized multi-walled carbon nanotubes
11:07	Avital Horowitz	C. Moraes	• Quantifying the Biomechanics of Idiopathic Pulmonary Fibrosis
11:20	Maryam Abdollahi Neisiani	C. Chilian and J. Chaouki	• Quantifying Rare Earth Element Content in Chemical Separation Processes by Neutron Activation Analysis
11:33	Thomas Vlasic	A. Rey and P. Servio	• Compressibility and Equations of State of Structure II Gas Hydrates
11:46	Sanchari Biswas	A.-M. Kietzig	• Effects of irradiation parameters in femtosecond laser micromachining of metals
11:59	Jason Ivall	P. Servio	• Liquid-Phase Convective Currents during the Melting of Ice Droplets Containing Water and Multiwall Carbon Nanotubes
12:15	**Lunch break**		

Session 2 -Track B: Ballroom B

Start*	Name	Supervisors	Title
14:15	Paul Westlund	V. Yargeau	• Examining the Impact of Ozonation on Endocrine Activity of Pesticides Using Yeast Based Bioassays
14:28	Oscar Matus Rivas	A. Rey	• Molecular dynamics investigation of the self-assembly mechanism in lyotropic chromonic liquid crystals
14:41	Sary Sarkis	C. Hoesli	• Mouse pancreatic cells encapsulated in alginate with silica nanoparticles
14:54	Marc-Antoine Campeau	R. Leask	• Development of a realistic intracranial aneurysm in vitro model for cell culture to study the impact of hemodynamic forces on aneurysmal tissue
15:07	Linda Balabanian	A. Hendricks	• The Role of the Microtubule Cytoskeleton in Regulating Intracellular Transport
15:20	**Coffee break**		

*Talks are 13 minutes in duration for graduate students including 3 minutes questions period.

Thank you for attending

Seminar Session

Session 3-Track B: Ballroom B

	Name	Supervisors	Title
15:35	Alexandre Milovanoff	R. Samson, C. Gaudreault, F. Cheriet	• Optimization of energy consumption in smart homes: A new LCA-based Demand Side Management program
15:48	He Li	G.S. Patience	• Optimization of $LiFePO_4$ wet media milling and regressive PBM modelling
16:01	Hawa Alajaili	S. Omanovic	• Corrosion Inhibitors for Cooling/Heating Water-based Systems
16:14	Jean-Michel Tucny	F. Bertrand	• Prediction of the Impact of Fiber Polydispersity on Filter Efficiency
16:27	Mahesh Edake	G.S. Patience	• Gas phase hydrogenolysis of glycerol to 1, 3-propanediol in a fluidized bed
16:40	**Poster session / Wine and cheese**		

*Talks are 13 minutes in duration for graduate students including 3 minutes questions period.

Thank you for attending

Poster Session

Main Hall

Name	Supervisors	Title
Hajer Rokbani	A. Ajji	• Study of the Rheological behavior of PLA and ZnO based solutions for electrospining process
Ling Tao	J. Chaouki and L. Martinu	• Investigation of the solid-state reaction of $Li_4Ti_5O_{12}$ for lithium-ion batteries anode material
François Picard	J. Chaouki	• Oxidation of heavy metal and petroleum contaminated soils with sodium hypochlorite
Christine Pu	N. Tufenkji	• Environmental fate and transport of transition metal dichalcogenide nanosheets
Anikke Rioux	R. L. Leask	• Immunohistochemistry of the Ascending Aorta (with Alexander Emmott)

*Posters are to be installed at 16:00 in Main Hall

Thank you for attending

Plenary lecture #1

Improving resource efficiency to address climate change by observing Nature

Dr. Jocelyn Doucet, P. Eng., Ph. D CEO Pyrowave

This presentation will discuss the climate change challenge and how it needs to be addressed by closing the resource loop. More specifically, a parallel will be drawn between what we do since the beginning of the industrial era and what nature can teach us on addressing waste recovery. We will see that nature, by design, reutilizes all the resources since the resources on the planet are finite: there is no incoming feed of new material from the Universe to replace what is consumed. However, energy is abundant, free and available everywhere through solar radiation. This is why evolution was more favorable to systems that could work together at recycling all atoms, without primarily favoring energy efficiency of those systems. This is in direct contrasts with our industrialized world where energy has a cost, because it is resource–derived, which forces us to be primarily energy efficient. In most case, recovering waste requires work to reorganize the matter and our focus on energy efficiency discards right away any attempts or processes that would require energy to convert waste.

Billions of years of evolution show that the best and yet most efficient system for closing the loop of carbon requires energy and is called photosynthesis. Perhaps that tells us that the "holy grail" technology that everybody is looking for that would use minimal energy to recycle material might not be possible. Perhaps, that should guide our approach towards recycling.

So now that we admit that work is needed to recycle, what do we do? How does Nature approach the waste recovery from a process standpoint? We will observe the mechanism by which the waste is recovered and conclude that recycling occurs at the atomic or molecular level. Large structures, like celluloses, lignin, etc. are decomposed into smaller molecules. This happens through multiple reactions until the final molecules obtained are re-usable for protein or sugar synthesis. Furthermore, when we think of it, Nature operates in a distributed way: there is not only one big tree absorbing all the carbon dioxide, nor is there only on big worm able to digest the entire tree leaves from all trees around the globe. Treating waste locally at a small scale is essential as all the waste do not have the same composition and often require different approaches for degradation. It also avoids transportation of waste from the source to the treating site.

As an application example, we will talk about a recent successful industry-university collaboration incorporating lessons from Nature to address plastic waste recovery. We will introduce the Pyrowave technology that uses microwave assisted pyrolysis at small scale to form monomer and waxes from waste plastics. The unit therefore processes locally plastics and converts them into smaller molecules that are re-introduced into the polymer synthesis ecosystem to make new plastics. We will cover some key technical challenges that were addressed through the partnership and some applications.

Plenary lecture #2

Science and engineering of clathrate (gas) hydrates and applications in CO_2 capture and storage and safe hydrocarbon transportation.

Prof. Peter Englezos Chair and Professor, Department of Chemical Engineering, University of British Columbia

Gas hydrate or clathrate hydrate crystals are non-stoichiometric inclusion compounds. They form at suitable thermodynamic conditions, usually high pressure and near freezing temperature from water (*hos*t molecule) and *guest* molecules with suitable size such as CO_2, CH_4, C_2H_6, C_3H_8, H_2, and N_2. The guest molecules are accommodated inside well-defined cages of hydrogen-bonded water molecules (*host lattice*). Favorable gas hydrate formation conditions may be encountered during production, transportation and processing of hydrocarbons. Such conditions also exist in many places in the earth and thus hydrates of natural gas are found onshore, under the permafrost region of the earth and offshore, below the sea floor along the continental margins. While this natural gas, also known as *frozen energy*, represents a future resource it may also be a source of methane (a greenhouse gas) in the atmosphere if it is released in an uncontrolled manner (*runaway greenhouse effect*).

Capture of CO_2 from large point sources and the subsequent placement of captured CO_2 into a subsurface porous formation of the earth (geological storage) is considered an effective climate change mitigation strategy until the world's energy systems become non-fossil dependent. Depleted gas reservoirs are such an attractive formation because the fluid trapping mechanisms and the reservoir properties are known. The storage potential in the world's gas fields is estimated to be 520 Gt of CO_2. One example of underground storage of CO_2 is the Sleipner West gas field in the North Sea. Also, the Otway project in Australia demonstrated long-term storage in a gas field.

Clathrate hydrates may offer technology solutions along all aspects of carbon management. In this presentation a brief introduction to major milestones of gas hydrate science and engineering will be presented. This is followed by a discussion of recent results from our lab that contribute to a deeper understanding of the behaviour of clathrate hydrate systems. We focus on the interactions of hydrate crystals with additives employed to control nucleation and growth and also on the formation of nano-bubbles during hydrate dissociation. Hybrid conceptual processes for pre and post-combustion capture based on hydrate crystallization are also presented and the storage of CO_2 as hydrate in shallow natural gas reservoirs is also discussed.

Seminar Session- Ballroom A

10:15

Conversion of glucose to C-6 carboxylic acids

Authors: Davide Carnevali; Supervisors: G. S. Patience ; Affiliation: Polytechnique Montréal

Glucose is the most abundant sugar on Earth. Agricultural and forestry residues are important sources. Many innovations to add value to sugar rely on liquid phase batch processes and continuous flow reactors for the production of gluconic acid, levulinic acid, 2,5-furandicarboxylic acid or adipic acid. Here, for the first time, we report that glucose reacts in the gas phase. We atomized an aqueous solution of glucose into a fluidized bed reactor loaded with a bifunctional catalyst at 250˚C / 350˚C. Our target is to produce C-6 carboxylic acids such as adipic acid, 2,5-furandicarboxylic acid and gluconic acid. We loaded 5 g of catalyst to a 15 mm ID quartz tube, co-injecting a 5 %wt glucose aqueous solution with oxygen at different molar ratio. We sampled the products liquid quench at intervals for HPLC, GC and LC-MS analysis. An on-line MS estimated the non-condensable gas concentration at 3 Hz.

10:28

Validation of LuminoTox as a tool to monitor wastewater toxicity

Authors: Meghan Marshall; Supervisors: V. Yargeau; Affiliation: McGill University

Contaminants of Emerging Concern (CECs) such as pesticides, endocrine disruptors, and personal care products are present in the environment in nanograms to micrograms per milliliter concentrations. CECs end up in the environment mainly along with discharged treated wastewater. Adverse effects caused by chronic exposure to CECs are limited but of concern, thus, high throughput methods to monitor residual wastewater toxicity are required. LuminoTox, which measures the inhibition of photosynthesis, is used in to monitor water toxicity and could be used specifically for wastewater. The purpose of this work was to validate the LuminoTox as a tool to monitor the toxicity of secondary wastewater effluent. Five different wastewater characteristics were validated including conductivity, total organic content, chemical oxygen demand, colour, alkalinity and hardness, for ranges typical of secondary effluents. Principle component analysis was applied and it was determined that conductivity and colour have the most effect on the modification of toxicity measurements.

10:41

Development of an optimized-consequential life cycle assessment methodology and its application to the electricity generation sector

Authors: Hassana Elzein; Supervisors: J. Samson ; Affiliation: Polytechnique Montréal

Life cycle assessments currently face problems in the representation of time-dependent systems which operation can vary in time between hours, weeks or seasons. Usually, the calculation of life cycle environmental impacts is based on annually aggregated data representing industrial processes; however, the averaging of these data results in erred estimations of the environmental impacts and thus unreliable LCA results. Among time-variant systems, smart technologies are having an exponential growth and require a new LCA methodology to evaluate, compare and manage their environmental impacts. In this project, a new approach, the optimized-consequential-LCA using data collected in real-time is developed and applied to a smart-grid context. Firstly, an integration framework of energy storage systems to an electric grid is defined. Secondly, this framework is evaluated and optimized in real-time. Then, the environmental impacts of the resulting grid mix is compared to a business as usual situation.

10:54

Simulation of a Full Fuel Cell Membrane Electrode Assembly Using Pore Network Modeling

Authors: Mahmoudreza Aghighi; Supervisors: J. Gostick; Affiliation: McGill University

One of the main challenges for PEMFCs commercialization is understanding the numerous simultaneous transport processes within the porous electrodes. In general, the dynamic operation PEMFCs result in large humidity and temperature variations inside the cell, leading to liquid water condensation which significantly alters the transport processes in the porous electrodes. Understanding its effect on the cell performance has been a major goal of the PEM studies. In this work, a pore network model (PNM) was applied to both sides of a fuel cell membrane electrode assembly. This model required the development of an iterative algorithm to couple the numerous physical processes occurring during operation. It was shown that depending on the liquid water configuration in the porous electrodes, ohmic polarization might increase due to the local starvation of reactants. This work highlights the strength of PNM to resolve discrete water blockages in a PEMFC.

11:07

Chitosan/bacterial cellulose nanofibrous structures by coaxial electrospinning for wound dressing applications

Authors: Nury Ardila [a], Nelson Medina [a], Mounia Arkoun [a], Marie-Claude Heuzey [a], Abdellah Ajji [a], Chandra J. Panchal [b]; Supervisors: M.C. Heuzey and A. Ajji; Affiliation: [a]CREPEC, Department of Chemical Engineering, Polytechnique Montréal, [b]Axcelon Biopolymers Corporation

Chitosan and cellulose are two biopolymers with unique physicochemical and biological properties, including renewability, biocompatibility, abundance and biodegradability, which make them attractive for different applications. In particular, bacterial nanocellulose (BNC) is of interest in the medical sector owing to its regenerative properties in tissue engineering whilst the antimicrobial properties of chitosan are widely recognized. The combination of these two properties (regenerative and antimicrobial) can be of significant interest for the biomedical industry in the scope of new materials designed for wound dressing applications. However, despite their good properties, the processing of either cellulose or chitosan alone is limited since they are not thermoplastics nor soluble in most common solvents. In addition, their common processing becomes even more challenging if it is intended to use both materials together to take advantage of their individual properties. Therefore, the present research work aims at studying coaxial electrospinning for the production of nanofibrous structures containing both chitosan and bacterial nanocellulose. This technique consists in simultaneously spinning inner and outer solutions through a spinneret composed of two needles aligned concentrically to produce core-shell structured nanofibers. Our results showed that fiber formation may be obtained by using a blend of chitosan (CS) and poly(ethylene oxide) (PEO) as an inner aqueous acidic solution, and a DMAc/LiCl solution containing bacterial nanocellulose (BNC) as the outer layer. Electrospun CS/PEO/BNC fibers had a diameter of 85 nm on average, and a narrow fiber size distribution. The core/shell structure was examined using transmission electron microscopy (TEM). In addition, energy-dispersive X-ray spectroscopy (EDS) analysis showed that nanofibers contained both CS and BNC along their structure. Finally, the antimicrobial properties of the mats were investigated against a non-pathogen strain of E. coli and a decrease of 99.9 % in bacterial population indicated that mats were providing adequate antimicrobial activity.

11:20

MWCNT/Pt composite electrode with reduced Pt loading for hydrogen evolution reaction

Authors: Remi Laraque; Supervisors: S. Coulombe and S. Omanovic ; Affiliation: McGill

In the attempt to develop greener energy alternatives, hydrogen-based technologies are in a prime position. However, most hydrogen gas is still produced by the reforming of fossil fuels. As an alternative commercial electrolyzers coupled to a renewable energy source have the ability to produce high purity hydrogen in a zero greenhouse-gas-emission process. The platinum catalyst in polymer-electrolyte-membrane-based electrolysers remains the costliest component.
In this talk, I will present the development of a composite electrode with reduced platinum loading while maintaining good catalytic performance. Chemical vapor deposition followed by pulsed laser deposition are used to produce multiwall carbon nanotubes decorated with platinum nanoparticles. The platinum loading is in the range of 0.02-0.4 mg.cm-2. The current density achieved at an overpotential of η=-0.1 V ranges from 100 to 400mA mA cm-2. In addition, testing has shown that these electrodes are highly stable during extended periods of operation. Therefore, it can be concluded that the produced electrodes exhibit very high catalytic activity towards hydrogen production even at reduced platinum loading.

11:33

Design and Characterization of Surface Modified microparticles with stimuli-sensitive and reversible aggregation/disaggregation behavior

Authors: Faezeh Sabri; Supervisors: N. Virgilio, J.R. Tavares, and L. Fradette; Affiliation: Polytechnique Montréal

Controlling particles aggregation and disaggregation properties can be a key step in separation processes involving complex fluids comprised of immiscible liquids and micro/nanoparticles, such as solid-stabilized (Pickering) emulsions. These fluids are encountered in various industries such as petrochemistry and metallurgy, waste water treatment, the food and cosmetics fields, and emerging technologies like microreactors and stimuli-sensitive drug delivery devices. The separation of the liquid and solid phases is often an energy intensive process, and the design of facile, efficient and ecofriendly methods is needed to improve and enhance the existing technologies. This project aims at developing a new technique to facilitate the aggregation of particles and separation of complex fluids constituents in Pickering emulsions. Our approach is based on the design and synthesis of surface modified micro/nanoparticles with stimuli-sensitive and reversible aggregation/disaggregation properties. Model systems based on silica and glass micro- and nanoparticles, functionalized with a pH sensitive polysaccharide, have been developed and show reversible aggregation/disaggregation properties in aqueous solutions. The mechanism is explained based on zeta potential measurements and the formation of hydrogen bonds between the grafted polysaccharide chains.

11:46

Measurement and prediction of removal of contaminants of emerging concern during wastewater treatment

Authors: Zeina Baalbaki; Supervisors: V. Yargeau; Affiliation: McGill University

The occurrence of contaminants of emerging concern (CECs), including pharmaceuticals, illicit drugs and hormones in water bodies pose a risk on the aquatic environment and the quality of drinking water sources. This has alarmed scientists and engineers to develop improved methods to monitor these compounds. This study aims at obtaining reliable data on the fate of selected CECs within the treatment sequence to calibrate models of removal of CECs. Sampling was conducted at three WWTPs using an advanced sampling strategy that requires prior hydraulic modelling of each WWTP. The obtained hydraulic models for the three WWTPs were significantly different leading to different sampling and calculations strategies to determine reliable removal levels, which further demonstrates the importance of hydraulic modelling in CEC removal studies. The modelling software WEST was subsequently used to build a fate model that predicts the fate of selected CECs, and the experimental results were used for validation.

11:59

Gas phase oxidation of 2-methyl 1,3 propanediol to methacrylic acid over heteropolyacid catalysts

Authors: Mohammad Jaber Darabi Mahboub; Supervisors: G. S. Patience ; Affiliation: Polytechnique Montréal

The acetone cyanohydrin process to produce methyl methacrylate (MMA) relies on expensive and toxic feedstocks and suffers from low yield. Methacrylic acid (MAA) is an alternative feed but current processes are less economic that require multi steps and catalysts that carbonylate C1-C3 hydrocarbons have a short life time. Here we report alternative chemistry based on 2 methyl 1,3 propanediol (2M-1,3 diol) which is a co–product of the hydroformylation of alchohol to 1-4 butanediol. A cesium salt of the Keggin type heteropoly acid(HPA) partially oxidizes 2M-1,3 diol to MAA. Inserting vanadium into the HPA reduces the Mo6+ to Mo5+ and promoting it with copper increases selectivity to MAA but decreases conversion by 11%. The HPA catalyst operates in a gas phase fluidized bed in which a 0.3 mm nozzle atomizes a 2M-1,3 diol liquid feed into the bed at 250 C. The maximum selectivity to MAA and methacrolein (MAC) was 41% and 33%, respectively, at 63% conversion. In the first step the 2M-1,3 diol dehydrates to MAC, which then oxidizes to MAA. The main byproducts are methane (gas phase) due to decomposition of the reactant and 2–methyl propanal (liquid phase) because of hydrogen spillover of MAC.

14:15

In vitro and in situ study of antibacterial properties of electrospun chitosan-based nanofibers.

Authors: Mounia Arkoun; Supervisors: M.C. Heuzey and A. Ajji; Affiliation: Polytechnique Montréal

This study investigates the in vitro and in situ antibacterial properties of electrospun chitosan nanofibers (CNF) against Escherichia coli, Salmonella typhimurium, Staphylococcus aureus and Listeria innocua. Sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), agarose gel electrophoresis and β-galactosidase essay analysis are performed to highlight the effect of chitosan on membrane permeability. In situ analysis of contaminated meat packaged with and without (conventional meat packaging) CNF are also performed. Our in vitro experiments demonstrate that CNF significantly inhibit bacterial growth. The results of our microbiological analysis of contaminated meat packaged with CNF show a significant reduction (99.9%) of bacterial population. The results reveal that chitosan can interact with the bacterial cell membrane and cause leakage of intracellular components among which proteins, DNA and enzymes. Our results indicate that the release of such components to the extracellular medium is an indication of membrane permeabilization, as verified by transmission electron microscopy (TEM) observations.

14:28

Characterization of Silver Nanoparticles in Wastewaters and Understanding their Interaction with the Green Alga, Chlamydomonas reinhardtii

Authors: Agil Azimzada; Supervisors: N. Tufenkji and K.J. Wilkinson; Affiliation: McGill University

Despite the utility of silver nanoparticles (Ag NPs) as anti-bacterial agents, the 'nano-scale' properties of these nanoparticles raise potential exo-toxicological implications when they end up in the environment. Wastewater effluents represent one of the main routes through which Ag NPs can reach aquatic environments, such as lakes and rivers, where they may potentially interact with the aquatic life. In wastewaters, Ag NPs may undergo different chemical and physical transformations, which may alter the potential toxicity of these NPs towards aquatic organisms. The main objectives of our study are to characterize the Ag NPs in wastewater effluents and then assess their interactions with a model organism, the green alga Chlamydomonas reinhardtii. We are going to present the results that show the dissolution patterns of Ag NPs for different types of media; investigate the potential bioavailability of dissolved silver species and assess the bioavailability and uptake of Ag NPs by C. reinhardtii.

14:41

Preparation and Characterization of Thin Polymer-like Coatings on Silicon via Photo-Initiated Chemical Vapor Deposition (PICVD)

Authors: Donya Farhanian; Supervisors: J.R. Tavares and G. De Crescenzo; Affiliation: Polytechnique Montréal

Techniques for fabrication of functionalized polymer-based surfaces have been predominantly based on wet chemistry. Such solvent-based techniques suffer from the involvement of potentially toxic reagents, by-products and solvents, and often complex preparation methods. On the other hand, alternatives such as plasma-enhanced or thermally-assisted chemical vapor deposition require operation under vacuum and/or high-temperature compatibility. These drawbacks are a hindrance to scale-up and commercialization of these techniques for applications where there is no high added value. We propose an alternative, milder and low-cost approach: photo-initiated chemical vapour deposition (PICVD). This study explores the reaction kinetics of a binary precursor mixture composed of carbon monoxide (CO) and hydrogen (H_2) to deposit a polymer-like film on silicon wafer substrates. A germicidal UVC lamps (emitting at 253.7 nm) are used to illuminate a plug flow like quartz tube reactor. X-ray photoelectron spectroscopy (XPS) and profilometry were applied for chemical analysis and thickness measurements of the deposited films, respectively.

14:54

Development of Catalyst Coating for an Optically Accessible Plate Reactor

Authors: JingSi Jiang; Supervisors: J. Kopyscinski; Affiliation: McGill University

An optically accessible plate reactor provides opportunity for direct measurements of the temperature profile along the catalytic surface during a reaction, allowing more detailed investigation of reaction kinetics compared to traditional catalytic reactors with end-of-pipe measurements. The reactor requires a well-coated catalyst plate with a known catalyst mass distribution, and systematic studies are needed for a clear understanding of the choice of material and coating technology. This study aims to develop a procedure leading towards a strong and homogeneous catalyst coating, which will be then used to gain a deeper insight into the fundamental steps of an interested reaction (e.g., methanation). Particular interest was placed on pre-treating Fecralloy plates and subsequently coating the plates with aqueous or organic based slurries of commercial Ni catalyst using various techniques. Mechanical strength and height profile of the coatings were then investigated, and surface characterizations were performed to examine microscopic morphology and chemical composition.

15:07

Accounting for geographic variability and speciation in the terrestrial ecotoxicity of copper. Case study of wine consumption in Quebec, Canada

Authors: Ivan Viveros Santos; Supervisors: L. Deschênes, C. Bulle; Affiliation: Polytechnique Montréal

Copper-based fungicides are applied in vineyards leading to copper accumulation in soils. Current models in life cycle assessment (LCA) disregard the fact that metals can exist in various forms with different behaviour and toxicity depending on the soil properties. The objective of our study is to determine the importance of including copper speciation to the terrestrial ecotoxic impact using a LCA case study. The LCA of a bottle of wine consumed in Quebec was performed, using the IMPACT 2002+ methodology. Eleven scenarios were analysed according to the wine market share by country of origin. When using current characterisation factors (CFs), the ecosystem quality category was dominated by copper emitted to soil during the viticultural stage. Using CFs accounting for speciation and geographic variability let to a decrease of the copper contribution to the terrestrial ecotoxicity, from 98% to less than 1%. These results show the need to include metal speciation in LCA.

15:35

Electrochemical reduction of CO2 to low-molecular-weight organic molecules

Authors: Mahmoud Rammal; Supervisors: S. Omanovic; Affiliation: McGill University

As global warming directly affects the ecosystem and humankind in the 21st century, solutions are continuously being sought to reduce the emissions of greenhouse gases such as CO_2. To achieve this goal, several methods prove to be useful; among the available technologies electrochemical reduction of CO_2 is an emerging field that aims not only to reduce the levels of CO_2 but also to convert this undesirable product into value-added molecules. However, the process is complex and depends on several factors such as voltage, temperature, pressure and pH.
Electrochemical reduction of CO_2 into value-added products in an aqueous electrolyte was investigated using Ru and Ir/Ru mixed metal oxide coatings deposited on Ti. Under the investigated experimental conditions, the research has not yielded satisfactory evidence to ascertain the electrocatalytic activity of those coatings toward the conversion of CO_2 into valuable organic molecules dissolved in the liquid phase despite their favorable electrochemical properties.

15:48

Catalytic partial oxidation of methane over Pt/Rh catalysts supported on FeCralloy fibre

Authors: Zhenni Ma; Supervisors: G. S. Patience ; Affiliation: Polytechnique Montréal

Micro-Gas-to-Liquids technology (GtL) reduces flared natural gas and emissions while producing valuable diesel. Integrating a high pressure syngas step with Fischer-Tropsch (FT) in a single vessel reduces investment and operating costs to synthesize GtL liquids. Methane catalytic partial oxidation (CPOX) to produce syngas for FT is an economic opportunity for micro-refineries. Many metals and metal oxides selectively convert natural gas to CO and H_2 but they also form coke, which must be removed intermittently otherwise it deactivates the catalyst and fouls reactors and process lines. FeCralloy woven fibres are promising supports to partially oxidize methane because they resist high temperatures, are highly conductive, and can be molded into shapes. So far we successfully dispersed Pt and Rh over the surface of FeCralloy fibres that we coated Al_2O_3 and Al_2O_3/CeO_2 via in-situ pyrolysis spray and MgO via solution combustion synthesis. The selectivity to syngas of these catalysts was better than commercial Pt gauzes at 900 °C and from 0.1MPa and 2 MPa. Over Pt/Rh/MgO FeCralloy catalysts, at 2MPa and a residence time of 0.3 s, syngas yield was 50 % CO with a H_2/CO ratio of 2. All the oxygen was consumed for all experiments, which is critical for the FT step that requires reducing conditions.

16:01

CO_2 reduction on Pt-YSZ solid-oxide electrolysis cell

Authors: Charles Bruel; Supervisors: G. S. Patience ; Affiliation: Polytechnique Montréal

Carbon dioxide is a product of combustion and fermentation (sugar fermentation for alcoholic beverages, bioethanol production) and is the second most abundant anthropogenic gas (after water vapour) that contributes to the greenhouse effect. Electrolysis is one process that can reduce the amount of CO_2 rejected in the atmosphere as it activates the chemically stable CO_2 molecule. Yttrium stabilized zirconia (YSZ) cells conduct O_2- anions which may react CO_2 to methanol or CO. YSZ is an ionic promoter for Pt catalysts in the oxidation of CO and hydrocarbons such as propane (electrochemical promotion of catalysts - EPOC). Reversing the potential applied to the cell, we aim at reducing CO_2 into hydrocarbons in a single chamber reactor. The cell comprises a YSZ electrolytic disc with Pt nanoparticles electrodes deposited by LASER ablation. FE-SEM analysis of the electrodes outlined the morphology of the electrodes.

16:14

Graphene oxide-metal oxide composite catalyst support for alkaline fuel cells

Authors: Alison Fraser; Supervisors: J. Gostick and J. Barralet; Affiliation: McGill University

Alkaline fuel cells (AFC) are a highly efficient, clean technology for electricity generation. They have the key benefit of not requiring expensive platinum catalysts. In this work a graphene oxide-titanium dioxide composite catalyst support for use at the AFC cathode was synthesized using an ultrasonic phosphate bonding technique. Thermal gravimetric analysis was used to quantify the amount of graphene oxide in the composite. The surface area, particle size, and crystalline structure were investigated using gas sorption, scanning electron microscopy, and X-ray powder diffraction, respectively. Silver nanoparticles were deposited using one-step and two-step UV deposition techniques. Oxygen reduction reaction performance was tested in alkaline conditions. Ongoing work focuses extending the characterization including measuring the electrical conductivity using a novel 3D-printed device.

16:27

Enhancing the terrestrial ecotoxicological effect modeling of metals in life cycle impact assessment

Authors: Clara Tromson; Supervisors: L. Deschênes and C. Bulle; Affiliation: Polytechnique Montréal

In life cycle assessment, the effect factor of a metal in soils (EF) is extrapolated from aquatic ecotoxicological data by using a generic partition coefficient (Kd). This method does not account for the difference in sensitivity between aquatic and terrestrial organisms, or the variability of soil properties. Conversely, the toxicity of a metal depends on metal speciation, which varies depending on soil physicochemical conditions. This research estimates the influences of both metal speciation and soil properties on the value of the EF. For each type of soils, regionalized Kd are obtained with a speciation model (WHAM7). For zinc, EFs extrapolated using those Kds from aquatic ecotoxicological data vary by 6 orders of magnitude across soils. This new approach will be validated with terrestrial ecotoxicological measured data and compared to modeled EF accounting for cations competition via the terrestrial biotic ligand model. Regionalized EF will be determined once these extrapolations verified.

Seminar Session-Ballroom B

10:15

Effect of Heat and Water on the Stability of Plasma Polymers for Functionalization of Carbon Nanotubes

Authors: Larissa Jorge; Supervisors: S. Coulombe and P.-L. Girard-Lauriault; Affiliation: McGill University

Wrapping of surfactants or polymers onto carbon nanotubes (CNTs) is a common technique to prepare stable nanofluids (NF). We wish to present our results using plasma enhanced chemical vapor deposition (PECVD) of an organic layer onto CNTs by a dry process. CNTs are exposed to an RF plasma (13.56 MHz, 35 W) for 5 min. With a mixture of ethylene and ammonia or carbon dioxide, the deposited layer contains ~22 at% of nitrogen and ~22 at% of oxygen, respectively. In a nitrogen atmosphere, the organic layer is stable up to 150 oC and further heating degrades the layer until it has lost about two thirds of its original mass at 550 oC. Exposure to water causes oxidation of some of the functional groups. CNTs coated with these plasma polymers are stable in water.

10:28

Surface wetting and surface tension of stable and unstable carbon nanotube nanofluids

Authors: Adya Karthikeyan; Supervisors: S. Coulombe, A.-M. Kietzig; Affiliation: McGill University

Nanofluids - the engineered colloidal suspension of nanoparticles in base liquids - have captivated the interests of researchers for various scientific applications. Properties such as viscosity, thermal conductivity and surface tension of colloids differs from those of the base liquids. A rich literature explains that the properties of nanofluids vary from those of the base liquid and that this deviation is dependent on the concentration of the nanoparticles dispersed. However, the literature isn't clear on many fronts, and contradictory results are reported. The wettability and surface tension of nanofluids is a particular example where highly-conflicting results exist. Addressing this issue with stable multiwall carbon nanotube (MWCNT) nanofluids is the main scope of this contribution. Our experiments showed that surface tension and wettability remain constant for different concentrations of stable MWCNT nanofluids, however, it was observed that the contact angle varies for the agglomerated nanofluids and nanofluids stabilized with surfactants. Hence we conclude that the stability of nanofluids plays a key role in altering its wettability.

10:41

Catalyst preparation for fluidized bed reactors by spray drying

Authors: Nooshin Saadatkhah; Supervisors: G. S. Patience ; Affiliation: Polytechnique Montréal

Spray dried fluidized bed catalysts belong to the Geldart Group A and vary between 22 um to 200 um in diameter. Binder is either distributed throughout the particle with the active phase or surrounds the active phase as in a core-shell structure. We slurried WO_3/TiO_2 micronized powder with colloidal silica to form a slurry with a solid fraction of 5 % to 20 %. We varied the feed slurry concentration, binder concentration, slurry and drying air flow rates, two-phase nozzle pressure drop and inlet temperature. Most conditions only produced a very fine powder. The small particles were often fully spherical but we also produced large clusters that reached 150 um. The high pressure drop through the nozzle and low slurry concentration produced the fine powder. Particles agglomerated in the fluidized bed when we increased the slurry flow rate to the chamber such that the powder had not yet dried sufficiently.

10:54

Kinetics of carbon dioxide gas hydrates with the combination of tetra-n-butylammonium bromide and functionalized multi-walled carbon nanotubes

Authors: Jean-Sébastien Renault-Crispo; Supervisors: P. Servio and S. Coulombe; Affiliation: McGill University

Gas hydrates are crystalline structures of water that enclathrate gas molecules. Applications of interest for gas hydrate promotion include gas transport, storage and separation. Slow nucleation and kinetics have prevented larger scale use of hydrate technologies. A method to address these issues is to use additives to either shift the thermodynamic equilibrium to a more favorable state or to improve the kinetic rates of hydrate formation. In this study, a combination of tetra-n-butylammonium bromide (TBAB), a thermodynamic promoter, and functionalized multi-walled carbon nanotubes (CNTs), a kinetic promoter, is used to study the growth behavior of carbon dioxide gas hydrates. The addition of CNTs promoted the dissolution of the gas into the liquid phase. CNTs also helped reduce the time required for the hydrates to form, also known as the induction time. Despite these differences, CNTs appear to have no effect on TBAB hydrate growth rate.

11:07

Quantifying the Biomechanics of Idiopathic Pulmonary Fibrosis

Authors: Avital Horowitz; Supervisors: C. Moraes; Affiliation: McGill University

Idiopathic pulmonary fibrosis (IPF) is a chronic and fatal disease characterized by progressive stiffening of the lung matrix. IPF is perpetuated by pathologically activated fibroblasts that are significantly more contractile than normal lung fibroblasts (NLFs), however the underlying mechanisms of IPF remain poorly understood. Our objective in this work is to quantify the dynamics of healthy and diseased primary fibroblast cell-matrix interactions in physiologically-realistic, but precisely-defined culture systems. Results from a collagen contraction assay indicated that NLF and IPF cells were indistinguishable in terms of contractile remodelling in the presence of fetal bovine serum. In contrast, serum-free culture showed marked increases in contractile activity for IPF patient samples. Similar trends were not seen in single-cell traction force microscopy, suggesting different regulation on the single-cell and whole-tissue level. Understanding the biomechanics underlying IPF disease progression will provide insight to potential drug targets and therapies.

11:20

Quantifying Rare Earth Element Content in Chemical Separation Processes by Neutron Activation Analysis

Authors: Maryam Abdollahi Neisiani; Supervisors: C. Chilian and J. Chaouki; Affiliation: Polytechnique Montréal

The rare earth elements (REEs) are the fifteen lanthanide elements as well as scandium and yttrium with atomic numbers of 21 and 39. The increasing number of applications of rare earth elements in various industries has led to a growing interest in developing techniques for extracting these elements. A reliable and accurate characterization technique is needed to determine the concentration of the REEs at each step of the separation process. Neutron activation analysis (NAA) is a common technique for analyzing solid samples containing minerals. However, there are major challenges when analyzing samples with high concentration of rare earth elements. The aim of this work is to improve the NAA method for detecting the rare earth elements in batches of samples resulting from physical and chemical refining steps of REEs. When analyzing high concentrated samples, neutron self-shielding and gamma-ray attenuation effect are among the major challenges. By improving the detection geometry and employing iterative correction calculations, the accuracy of the results was 7% or better which was validated by certified reference materials.

11:33

Compressibility and Equations of State of Structure II Gas Hydrates

Authors: Thomas Vlasic; Supervisors: A. Rey and P. Servio; Affiliation: McGill University

Gas hydrates are crystalline solids composed of a network of hydrogen-bonded water molecules forming cage-like structures where small non-polar gas molecules (e.g. methane) or volatile liquids (e.g. neohexane) are trapped within. The material properties of gas hydrates are of fundamental importance to virtually all of their applications including flow assurance, natural gas transport and storage, hydrate formation models, and hydrate recovery from natural deposits. Despite their importance, gas hydrate properties are not well characterized in current literature. This work involves the use of density functional theory to determine the mechanical properties of structure II (sII) gas hydrates such as equilibrium lattice volume, bulk modulus, and the first pressure derivative of the bulk modulus. From these results, some well known equations of state (EOS) for solids (Murnaghan, Birch-Murnaghan, Vinet, Liu) were analyzed and compared. These EOS can then be used to characterize the compressional behaviour of sII gas hydrates.

11:46

Effects of irradiation parameters in femtosecond laser micromachining of metals

Authors: Sanchari Biswas; Supervisors: A.-M. Kietzig; Affiliation: McGill University

In the field of femtosecond laser micromachining of metals, most studies that report the effect of repetition rate compare the ablation threshold of metals micromachined at kHz range with MHz range and observe a decrease in the ablation threshold with an increase in repetition rate. However, these ranges are very wide and the trend in between these ranges are unclear. We present a comparison of the microstructure formation in Ti and Cu, micromachined at 1 and 10 kHz repetition rate. In Cu, a reduction in the ablation threshold was observed with an increase in repetition rate, which is similar to what has been reported previously. However, in Ti, the ablation threshold was observed to increase with an increase in the repetition rate, indicating a significant variation from earlier results. We propose that the metal-dielectric phase transition in Ti is responsible for showing higher ablation threshold at 10 kHz. Due to low thermal conductivity and high resolidification time the melt stays longer during which it acts as a liquid dielectric for the subsequent pulses, thereby increasing the ablation threshold.

11:59

Liquid-Phase Convective Currents during the Melting of Ice Droplets Containing Water and Multiwall Carbon Nanotubes

Authors: Jason Ivall; Supervisors: P. Servio; Affiliation: McGill University

The phase change of water droplets is a fundamental phenomenon with a wide range of applications. Myriad studies have examined both the evaporation and freezing processes of sessile droplets and characterized fluid motions within the liquid phase resulting from phase transformation. Interestingly, the literature available surrounding flow patterns within the liquid phase during the melting process are relatively scarce. In these experiments, solid sessile water droplets containing water or multiwall carbon nanotubes are thawed at ambient conditions on a Teflon/copper substrate and the liquid phase is characterized by visual inspection. The phase transition creates rapid fluid currents below the ice where the liquid rises along the outside of the droplet at the air-liquid interface and descends in the center of the liquid, producing a toroidal convection pattern. At the completion of melting, this mixing stops completely. The convective cells arise from a thermocapillary-driven mechanism due to temperature gradients imposed by the ice.

14:15

Examining the Impact of Ozonation on Endocrine Activity of Pesticides Using Yeast Based Bioassays

Authors: Paul Westlund; Supervisors: V. Yargeau; Affiliation: McGill University

The presence and persistence of contaminants in the environment is a rising concern both in terms of potential impacts on public health and aquatic organisms. Understanding the extent of toxicity risks from the exposure of these contaminants is far from complete and mechanisms regarding their transport and fate throughout the environment remain largely unknown. Due to the substantial volume of use in various industries, pesticides account for a large percentage of contaminants of emerging concern that are found throughout the environment including wastewater treatment plants. In order to effectively monitor the fate and biological activity of pesticides in wastewater a combination of chemical analysis and bioanalytical techniques are performed. Two yeast based bioanalytical techniques, which measure estrogenic and androgenic activity, are used to determine the effectiveness of advanced oxidation process for the removal of endocrine activity of pesticides in wastewater.

14:28

Molecular dynamics investigation of the self-assembly mechanism in lyotropic chromonic liquid crystals

Authors: Oscar Matus Rivas; Supervisors: A. Rey; Affiliation: McGill University

Lyotropic chromonic liquid crystals (LCLC) are anisotropic structures formed by spontaneous aggregation of non-amphiphilic sulfonated polyaromatic dyes dissolved in water. Most LCLC molecules assemble into stacks of varying size depending on many conditions such as temperature, concentration and pH. LCLC self-assembly process has been confirmed by X-ray diffraction and polarized UV-vis spectroscopic measurements. More recently, molecular dynamics simulations have been employed to untangle LCLC self-aggregation phenomena. Lately, LCLC have been utilized as precursors to synthesize vertically aligned graphene sheets. This method, which represents a novel chemical-mechanical synthesis route for graphene monolayers, needs to be thoroughly understood. Therefore, we present a methodology for studying the self-assembly process of Sunset Yellow dye and Disodium Cromoglycate anti-asmatic drug using molecular dynamics approach. Our objective is to shed light on the isodesmic aggregation mechanism of SSY and to simulate the first stages of the formation of vertical aligned graphene structures from chromonic mesogens.

14:41

Mouse pancreatic cells encapsulated in alginate with silica nanoparticles

Authors: Sary Sarkis; Supervisors: C. Hoesli; Affiliation: McGill University

Type 1 diabetes is characterized by the autoimmune destruction of the insulin-producing pancreatic β-cells. For diabetic patients, blood glucose monitoring and insulin injection is the predominant therapy. Islet transplantation has emerged as an alternative long-term treatment for diabetes, but this clinical option is limited by the need for lifelong immunosuppression to avoid graft rejection. To reduce immunosuppression requirements after transplantation, the islets can be encapsulated in an immunoprotective biomaterial (e.g. alginate gels). Islets encapsulated in hydrogels are typically infused into the peritoneal space. This method leads to variability in the islet distribution in the peritoneal cavity, hence in islet oxygenation and survival. The location of the encapsulated islets can be monitored in vivo through Magnetic Resonance Imaging (MRI). To induce a significant contrast between alginate-encapsulated islets and the surrounding tissues, paramagnetic gadolinium-labeled mesoporous silica nanoparticles (MSNs) can be used as positive MRI contrast agents. These MSNs exhibit strong relaxometric properties, they are very efficient "positive" MRI contrast agents, and they can also be effectively integrated in and sequestrated by hydrogels. Mouse insulinoma 6 (MIN6) beta cells were encapsulated in the presence or absence of MSNs to determine the effects of the MSNs on cell survival and cell growth. The cell growth rate was determined by measuring the change in packed cell volume over the course of two weeks. No significant differences between the growth rates of cells encapsulated alone or co-encapsulated with the MSNs were observed. Live/dead fluorescence imaging confirmed that the MSNs were not cytotoxic. The effect of the MSNs on beta cell gene expression is now being investigated. These studies will aid in improving encapsulated islet monitoring and performance after transplantation by means of a biomedical imaging modality that can be translated into clinical practice.

14:54

Development of a realistic intracranial aneurysm in vitro model for cell culture to study the impact of hemodynamic forces on aneurysmal tissue

Authors: Marc-Antoine Campeau; Supervisors: R. Leask; Affiliation: McGill University

Intracranial aneurysm rupture causes cerebrovascular hemorrhage which results in sudden brain function loss. The mechanisms underlying rupture are still poorly understood but inherently a mechanical failure. Risk factors linked to mechanical load, e.g. wall shear stress (WSS) have been proposed. Although aberrant WSS and atypical morphologic factors have shown to correlate with rupture occurrence, the mechanobiology remains unclear. It is hypothesized that cellular response triggered by forces exerted on the arterial tissue causes vessel wall mechanical failure.
In order to study this cellular response, a geometrically realistic intracranial aneurysm in vitro model has been developed and tailored for endothelial cell culture. The model provides scaffold for cells while exposing them to physiologically relevant flow. The manufacturing process consists in 3D printing of the vasculature and lost-wax casting using sugar alcohol. Preliminary results have shown that cells respond well to the model surface and the WSS gradient in the aneurysm.

15:07

The Role of the Microtubule Cytoskeleton in Regulating Intracellular Transport

Authors: Linda Balabanian; Supervisors: A. Hendricks; Affiliation: McGill University

The motor enzymes kinesin and dynein convert the chemical energy from ATP hydrolysis into mechanical work to move organelles and vesicular cargoes along the microtubule cytoskeleton in the cell. In addition to serving as tracks for transport, the microtubule cytoskeleton regulates the activity of motor proteins through the architecture of the network, microtubule-associated proteins (MAPs) and tubulin post-translational modifications (PTMs). However, it is not well understood how these factors influence motor motility, likely due in part to their interdependencies. For example, the MAP tau strongly inhibits kinesin-1 motility in purified systems, yet kinesin-1 drives long-range transport in neuronal axons where microtubules are heavily decorated with tau. To examine the influence of the cytoskeleton on motor protein motility, we isolated intact, native microtubule networks from cells and tracked the motility of single fluorescently-labeled motor proteins with high resolution using Total Internal Reflection Fluorescence (TIRF) microscopy.

15:35

Optimization of energy consumption in smart homes: A new LCA-based Demand Side Management program

Authors: Alexandre Milovanoff; Supervisors: R. Samson, C. Gaudreault, F. Cheriet; Affiliation: Polytechnique Montréal

Smart technologies such as smart metering are believed to play a significant role to provide new alternatives for sustainability. Energy management systems of smart buildings will offer new flexibilities in the grid with demand side management programs (DSM). DSM aims to enhance the integration of intermittent renewable energy sources and mitigate the generation by conventional power plants through changes in consumption patterns. In this work, environmental indicators based on life cycle assessment are established to provide a more comprehensive, sustainable and relevant pattern of electricity use. Innovative aspects of these indicators include the consideration of electricity imports and exports in the real time environmental profile of regional electricity and the short term consequences of power demand changes through the identification of dynamic marginal technologies. An optimization model is built with these environmental indicators and is compared with a financial incentive based model.

15:48

Optimization of LiFePO4 wet media milling and regressive PBM modelling

Authors: He Li; Supervisors: G. S. Patience ; Affiliation: Polytechnique Montréal

The raw material cost of LiFePO4 (LFP) for the cathode of lithium-batteries is lower than cobalt-based cathodes but LFP has poorer ionic and electronic conductivity. Reducing the particle size to submicron- or even nano-size improves its efficiency. Consequently, grinding energy and throughput are critical to maintain the material cost advantage. Here, we report the aqueous grinding performance of LFP powder in a wet media mill (Netzsch Minifer). The d50 of the initial powder was 27 μm (Horiba LA950) and the final target d50 was in the submicron range. We adopted an experimental design based on the Taguchi method to identify the optimum operating conditions in the range: LFP loading (0.20-0.30), milling media size (yttria-stabilized zirconia – YSZ – 0.3-0.5 mm), surfactant-to-LFP ratio (Tween-20 0-2 in arbitrary units), mill agitator rate (40-80 Hz). With 0.30 LFP loading, 0.3 mm YSZ media, a surfactant-to-LFP ratio of 2 and a mill rotation rate of 60 Hz, the Minifer achieved a specific throughput of 1.246 relative to the average of the source tests. Under these conditions, the effective grinding energy was 0.302 relative to the source tests average.

16:01

Corrosion Inhibitors For Cooling/Heating Water-based Systems

Authors: Hawa Alajaili; Supervisors: S. Omanovic; Affiliation: McGill Uinversity

Corrosion control of metals is of technical, economical, and environmental importance. One of the most effective, practical and economical ways for prevention of metal corrosion is by corrosion inhibitors. Corrosion inhibitors often play an important role in water treatment systems, chemical manufacturing, heavy manufacturing, oil and gas exploration and production, petroleum refining, and processing industries where they have always been considered to be the first line of defence against corrosion. Corrosion inhibitors interfere with the corrosion mechanism in order to prevent or mitigate it. Determining the most effective corrosion inhibitor for a given environment is essential, therefore, inhibitors' cost, toxicity, availability and their friendliness to the environment should be taken into account. Here, we report on recent achievement in design and selection of inhibitors that are used in cooling and heating water systems.

16:14

Prediction of the Impact of Fiber Polydispersity on Filter Efficiency

Authors: Jean-Michel Tuucny; Supervisors: F. Bertrand; Affiliation: Polytechnique Montréal

Fibrous air filters are used in applications where air quality is important, notably in respirators and confined environment ventilation systems. To better predict the capture efficiency and permeability of filters, and thus design optimized high-performance air filters that satisfy HEPA and N95 standards, we have devised a 3-step modeling approach to simulate the flow and capture mechanisms of aerosols within virtual filters, the composition of which can be varied systematically. More recently, we have thoroughly studied the impact of polydisperse fibre size distributions. Using our simulation data, we propose a new semi-empirical model based on a modified version of the single-fibre theory, which takes into account the polydispersity of the fiber size distribution. An evaluation of this new model with carefully designed experiments will be carried out using model micron-sized glass fibers.

16:27

Gas phase hydrogenolysis of glycerol to 1, 3-propanediol in a fluidized bed

Authors: Mahesh Edake; Supervisors: G.S. Patience; Affiliation: Polytechnique Montréal

Glycerol is a potential feedstock to produce 1,3 propanediol (1,3-PDO), which is a valuable commercial polyester monomer. For the first time, we report the gas-phase glycerol hydrogenolysis to 1,3-propanediol over Pt/WO3/Al2O3 in a fluidized bed operating above 240 C and ambient pressure. Fluidized beds are ideal contactors for this reaction because the heat transfer rates are sufficiently high to vapourize the glycerol thereby minimizing its combustion and thermal degradation. The yield of 1,3-PDO approached 14% after 2h at 260 C. The major co-products were 1,2-PDO (18%) 1-propanol (28%) and 2-propanol (15%). In the first step glycerol dehydrates to acrolein, followed by rehydration to 3-hydroxypropanal and then hydrogenation to 1,3-PDO. By-product —acrolein, ethylene glycol, propane, and acetone— increased with increasing temperature.

Poster Session

Study of the Rheological behavior of PLA and ZnO based solutions for electrospining process

Authors: Hajer Rokbani; Supervisors: A. Ajji; Affiliation: Polytechnique Montréal

PLA nanocomposites with antibacterial properties are of high potential interest as food packaging biomaterials. The investigations carried out in this study include the rheological properties of solutions used for electrospinning the nanofibrous mats as well as, the morphological evaluation of the mats based on poly(D,L-Lactide) nanofibers loaded with different zinc oxide nanoparticles. A detailed rheological analysis of the solutions used for electrospinning was carried out in order to understand the achieved morphology and structure of nanofibers. The effect of ZnO nanoparticles was investigated for various PLA solutions and solvents. The polymer solutions were prepared at various loading level of ZnO: 0.4, 0.8, 1, 3 and 5 wt % to the weight of the polymer. Two solvent systems were used : trifluoroethanol and a mixture of dichloromethane/ trifluoroethanol (50:50 v/v). The PLA solutions with low loading level of ZnO nanoparticles showed higher viscosity (□) than the neat PLA. They also showed a maximum value of □ at 3 wt % content. Solutions containing more than 3 wt % ZnO exhibited a notable decrease in viscosity, which could be probably due to the PLA degradation. The morphological-characterization of the electrospun nanofibers was performed using scanning electron microscopy (SEM). The SEM images showed a network of smooth randomly oriented PLA nanofibers. ZnO agglomeration was observed on the surface of the nanofibers.

Investigation of the solid-state reaction of $Li_4Ti_5O_{12}$ for lithium-ion batteries anode material

Authors: Ling Tao; Supervisors: J. Chaouki and L. Martinu; Affiliation: Polytechnique Montréal

Spinel lithium titanium oxide ($Li_4Ti_5O_{12}$) is regarded as the most promising anode material for lithium-ion batteries due to its long cycling life, high safety performance, and fast charging property. Although $Li_4Ti_5O_{12}$ possesses many excellent properties, the higher price of nano-spinel $Li_4Ti_5O_{12}$ not only rises the cost of battery systems, but limits its application as well. The main reasons for its high cost are attributed to the high synthesis temperature and complicated processes of solid-state reaction synthesis which is considered as the most suitable method for the large-scale production. Clear understanding of the fundamentals of the synthesis process is very important to control production conditions, minimize the energy consumption and lower synthesis cost. We investigated the kinetics of solid-state reaction between TiO_2 and Li_2CO_3 and found that tailoring the particle size of TiO_2 could decrease the synthesis temperature.

Oxidation of heavy metal and petroleum contaminated soils with sodium hypochlorite
Authors: François Picard; Supervisors: J. Chaouki ; Affiliation: Polytechnique Montréal

The project investigates the contribution of sodium hypochlorite (NaClO) in the remediation of real petroleum and heavy-metal contaminated soils. A soil treatment center provided the soil samples for this project. NaClO is scarcely reported in the literature on soil remediation although it is commonly used in pedogenic studies. The research innovates because of this novelty. Results report how the oxidation performance is affected by operating parameters and how the performance can be maximized. In particular, the results show how the resistance to oxidation caused by the natural soil organic matter can be overcome. This result is mostly relevant to heavy-metal soil remediation. This project is currently at a scale-up phase and selected technical informations on the scale-up are provided. A electrolysis unit generates in-situ the NaClO in the scale-up of this project. This technology transfer governs future works.

Environmental fate and transport of transition metal dichalcogenide nanosheets
Authors: Christine Pu; Supervisors: N. Tufenkji; Affiliation: McGill University

Transition metal dichalcogenides (TMDs) are nanosheets of transition metals sandwiched between two layers of chalcogens. Due to their direct electronic band gap, superior theoretical capacitance and exceptionally large specific surface area, TMDs are finding applications in optoelectronics, batteries and super-capacitors. Given their near future industrial-scale production, it is crucial to evaluate their environmental fate and impact due to potential release of these nanomaterials into aquatic environments. In this work, we investigate the transport and deposition of MoS_2 and WS_2, two major TMDs, in model groundwater environments. Using quartz crystal microbalance with dissipation monitoring (QCM-D) we demonstrate that the attachment of nanosheets to model aquifer grains (i.e., silica) is governed by DLVO theory. Furthermore, X-ray photoelectron studies reveal that the nanosheets undergo chemical transformation in various water chemistries.

Immunohistochemistry of the Ascending Aorta
Authors: Anikke Rioux, Alexander Emmott; Supervisors: R. L. Leask; Affiliation: McGill University

Most people are born with an aortic valve that has three leaflets, tricuspid aortic valve (TAV). However, 1-2% of the population are born with a congenital condition called bicuspid aortic valve (BAV) which causes these individuals to have only two leaflets. These individuals are more likely to develop aneurysms and aortic dissections. Matrix Metalloproteinase 2 (MMP2) is a protein that degrades elastin; this could be a major contributing factor to the formation of aortic dissections and aneurysms. This study relates the expression of MMP2 in aortic tissue of BAV patients in the inner curvature and outer curvature of the aorta using immunohistochemistry.