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POLYTECHNIQUE MONTRÉAL

LE GÉNIE EN PREMIÈRE CLASSE

Département de génie chimique

McGill

Department of Chemical Engineering

Journée de la recherche en génie chimique

Chemical Engineering Research Day

Mercredi le 15 mars 2017
8h30 – 18h00
Polytechnique Montréal
Pavillon principal
Amphithéâtre Bell (C-631)

Wednesday March 15, 2017
8:30 AM – 6:00 PM
Polytechnique Montréal
Main building
Bell Amphitheater (C-631)

https://mcgill.ca/chemeng/research-day

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General Program

8:30	Arrival/Registration
8:45	Welcome message
9:00	Plenary lecture: Prof. Robert Hayes, P.Eng, Department of Chemical and Materials Engineering, University of Alberta
10:00	Presentations (Parallel sessions – C-631 and B-600.16)
11:05	Coffee Break
11:20	Presentations (Parallel sessions – C-631 and B-600.16)
12:30	Lunch break (1st floor - rotonde)
13:30	Plenary lecture: Prof. Mario Jolicoeur and Mr. Philippe Leclerc, Department of Chemical Engineering, Polytechnique Montréal
14:15	Presentations (Parallel sessions – C-631 and B-600.16)
15:20	Coffee break
15:35	Presentations (Parallel sessions - C-631 and B-600.16)
16:40	Plenary lecture: Prof. Gregory S. Patience and Prof. Daria C. Boffito, Department of Chemical Engineering, École Polytechnique de Montréal
17:00	Poster Session + Wine & Cheese (Galerie Rolland – B-600.16)

Plenary lectures will be in the Bell Amphitheater (C-631)

Bell Amphitheater (C-631) & Galerie Rolland (B-600.16)

École Polytechnique de Montréal

2900 Edouard Montpetit Blvd

Chairs:

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

McGill University: Profs. Christopher Moraes and Corinne Hoesli

*Presentations are 13 minutes in duration for graduate students including 3-minute question periods.

Seminar Sessions

Track A: Bell Amphitheater (C-631) – Session 1

Time	Presentation #	Name	Supervisor(s)	Title
9:00	Plenary lecture			
	Prof. Robert Hayes, Department of Chemical and Materials Engineering, University of Alberta			Multi-scale modelling of structured catalytic reactors
10:00	1A	Paul Louyot	D.C. Boffito	Ultrasound process for Fischer-Tropsch iron catalyst synthesis
10:13	2A	Meghan Marshall	V. Yargeau	LuminoTox: A tool to monitor contaminants of emerging concern in secondary effluents and to evaluate their toxicity removal during ozonation
10:26	3A	Ray Tran	C. Hoesli & C. Moraes	A biomimetic approach to study the role of tissue shape on pancreatic stem cell differentiation
10:39	4A	Michael Wood	A. Kietzig	Development of a millimetric droplet generating apparatus
10:52	5A	Hajer Rokbani	A. Ajji	Rheological properties of the Poly(D.L-Lactide) solutions added with metal oxide nanoparticles
11:05	Coffee Break			
11:20	6A	Pardis Rofouie	D. Pasini & A. Rey	Surface pattern formation in plant-based plywoods and biological liquid crystal membranes
11:33	7A	He Li	G.S. Patience	Ultrasound assisted wet stirred media mill of high concentration $LiFePO_4$ catalysts
11:46	8A	Francois-Johan Chassaing	V. Yargeau	Development of a novel ozonation system for wastewater disinfection and removal of CECs
11:59	9A	Alexander Emmott	R. Leask	Using transesophageal echocardiographic strain imaging to predict the biomechanical properties of ascending aortic aneurysms
12:12	10A	Ahmad Khan	P. Servio & M. Maric	Ice and hydrate adhesion on poly(N-vinylcaprolactam) surfaces
12:30	Lunch Break (1st floor - rotonde)			

*Presentations are 13 minutes in duration for graduate students including 3-minute question periods.

Track A: Bell Amphitheater (C-631) – Session 2

Time	Presentation #	Name	Supervisor(s)	Title
13:30	Plenary lecture			
	Prof. Mario Jolicoeur and Mr. Philippe Leclerc, Department of Chemical Engineering, Polytechnique Montréal			Chemical Engineering and Beer-Making
14:15	11A	Christine Beaulieu	F. Bertrand & J. Chaouki	Understanding granular segregation mechanisms in a horizontal drum: numerical study with DEM
14:28	12A	Ali Aljishi	J. Kopyscinski	Ni-Ordered mesoporous catalyst for CO_2 methanation
14:41	13A	Zhenni Ma	G.S. Patience	FeCralloy® partially oxidizes methane to syngas selectively
14:54	14A	Basant Elsiwi	M. Maric & R. Leask	Diheptyl succinate (DHPS) – a really green plasticizer
15:07	15A	Oscar Marin	P. Servio	Phase equilibrium and liquid mole fraction measurements of tetra-n-butylammonium chloride + CO_2/CH_4 semi-clathrates
15:20	Coffee Break			
15:35	16A	Adya Karthikeyan	S. Coulombe & A. Kietzig	Carbon nanotube nanofluid-metal interaction
15:48	17A	Hicham Alayan	M. Maric & R. Leask	Properties of bioplastics made from poly(hydroxyalkanoate) (PHA) resins
16:01	18A	Wontae Lee	C. Moraes & R. Leask	Dispersible hydrogel mechanosensors to measure cell-generated stress within 3D cultures
16:14	19A	Nariman Yousefi	N. Tufenkji	Hierarchically porous graphene oxide-cellulose nanocrystal sponge for water treatment
16:27	20A	Nooshin Saadatkhah	G.S. Patience	Flame-assisted spray pyrolysis (FASP) hollow shell C-$LiMn_2O_4$ from aqueous solution
16:40	Plenary Lecture			
	Prof. Gregory S. Patience and Prof. Daria C. Boffito, Department of Chemical Engineering, Polytechnique Montréal			Intellectual Involvement merits Authorship
17:00	Poster session/Wine and cheese Galerie Rolland (B-600.16)			

*Presentations are 13 minutes in duration for graduate students including 3-minute question periods.

Track B: Galerie Rolland (B-600.16) – Session 1

Time	Presentation #	Name	Supervisor(s)	Title
9:00	Plenary lecture - Prof. Robert Hayes (Bell Amphitheater)			
10:00	1B	Marco Giulio Rigamonti	G.S. Patience	Spray dried VPP: core-shell morphology and attrition resistance
10:13	2B	Marlon Bustos	M. Maric	Effect of calcium carbonate on the mechanical properties of poly(hydroxyalkanoate) /green plasticizer blends
10:26	3B	Ipsita Bordoloi	S. Omanovic	Inhibition of carbon steel corrosion in closed-loop water-heating systems by using sodium caprylate as an environmentally-friendly corrosion inhibitor
10:39	4B	Evelyne Kasparek	P.L. Girard-Lauriault, M. Wertheimer & J.R. Tavares	Fabrication and characterization of photo- and plasma-chemically deposited sulfur rich thin films
10:52	5B	Mohammad Jaber Darabi Mahboub	G.S. Patience	Transient methacrylic acid selectivity study with calcination temperature; correlation of catalyst structure and reaction mechanism
11:05	Coffee Break			
11:20	6B	Stephanie Mok	C. Moraes	Measuring local 3D tissue stiffness using microengineered smart material probes
11:33	7B	Sara Babaei	P.L. Girard-Lauriault	The effect of surface chemistry and protein adsorption on monocyte adhesion to plasma deposited functional organic coatings
11:46	8B	Liji Le	R. Hill	Numerical calculation of gel electrophoretic mobility for “soft” spherical nanoparticles
11:59	9B	Francois-Julien Pelletier	P. Servio & P.L. Girard-Lauriault	Plasma-polymer coating reduces tetrahydrofuran hydrate adhesion
12:12	10B	Hassana Elzein	T. Dandres, A. Levasseur & R. Samson	Combining optimization and consequential life cycle assessment to investigate energy storage systems
12:30	Lunch Break (1st floor - rotonde)			

*Presentations are 13 minutes in duration for graduate students including 3-minute question periods.

Track B: Galerie Rolland (B-600.16) – Session 2

Time	Presentation #	Name	Supervisor(s)	Title
13:30	Plenary lecture – Prof. Mario Jolicoeur & Philippe Leclerc (Bell Amphitheater)			
14:15	11B	Sanya Siddiqui	C. Moraes & N. Tufenkji	The development of an in vitro co-culture device for bacterial infection studies
14:28	12B	Oscar Aguilar Gutierrez	A. Rey	Flow induced alignment of dilute collagen solutions in mixed flows for plywood formation
14:41	13B	Amin Sadeghi	J. Gostick & P. Servio	The interplay between pore structure and electrode performance: a pore network modeling study
14:54	14B	Shengnan Yan	G.S. Patience	Effect of particle pore size on RTD
15:07	15B	Madhuwanthi Buddhadasa	P.L. Girard-Lauriault & S. Lerouge	N-rich plasma polymer films to regulate fibrinogen adsorption
15:20	Coffee Break			
15:35	16B	Anne-Marie Boulay	M. Margni	The evolving concept of water scarcity and water footprint: when state-of-the-art and international consensus meet
15:48	17B	Emmanuel Nwanebu	S. Omanovic	Development of NiCo-oxide anodes for oxygen evolution in electrochemical hydrogen production by water electrolysis
16:01	18B	Yannick Essigan	G.S. Patience	Epoxy methyl as bio-plasticizers
16:14	19B	Philippe Leclerc	J. Chaouki & J. Doucet	Production of renewable styrene using catalytic microwave depolymerization
16:27	20B	Luke Matus	A. Kietzig	Laser chopper for downstream frequency reduction and pulse selection
16:40	Plenary lecture – Prof. Gregory S. Patience & Prof. Daria Boffito (Bell Amphitheater)			
17:00	Poster session/Wine and cheese Galerie Rolland (B-600.16)			

*Presentations are 13 minutes in duration for graduate students including 3-minute question periods.

Poster Session

Galerie Rolland (B-600.16)

Poster #	Name	Supervisor(s)	Title
1	Mitra Bahri	F. Haghighat & D. Rohani (Concordia)	Application of metal organic frameworks as dual functional adsorbent/catalysts for plasma air cleaners
2	Kieran Horry	D. Boffito & F. Galli	Bio-lubricant production using ultrasound and a heterogeneous catalyst
3	David Brassard	J.R. Tavares & M. Dubé	Heat dissipation in an electrically conductive nanocomposite
4	Kanayah Thumiah & Mohamad Kabbara	J.R. Tavares	Conception et analyse d'impact d'une usine de prétraitement de catalyseurs usés
5	Teresita Rode Garcia	X. Banquy	Effect of the preparation process on the architecture and the physicochemical properties of PLA-PEG nanoparticles
6	Ali Sahmoud	C. Moraes	McGill Chem-E Car Design Team

*Posters are to be installed between 16:30 and 17:00 in Galerie Rolland (B-600.16).

Plenary Lecture #1

Multi-scale modelling of structured catalytic reactors

Prof. Robert Hayes
Department of Chemical and Materials Engineering, University of Alberta

As the power of computers increases, and software becomes more sophisticated, advanced computational modelling is being increasingly used in many chemical engineering processes. including the modelling of heterogeneous catalytic reactors. If we disregard empirical type models, then the most common technique used to develop a computational reactor model is to develop the partial differential equations (PDE) that describe the conservation equations. Together with relationships for kinetics and physical properties, the PDE can be solved by the appropriate numerical method, usually the finite volume (FVM) or finite element (FEM) methods. Commercial software is often used.

The physical and chemical phenomena that are important in a catalytic reactor happen at several length scales. A model of a heterogeneous catalytic chemical reactor thus represents a multi-scale problem. The smallest scale that might be considered is the molecular scale, where the various molecules interact with active sites to effect the reaction. It is certainly common to eliminate this scale through the use of global kinetic expressions, however, it is often necessary to use more detailed mechanisms, either because the global approach lacks accuracy or a more detailed description of the product distribution is desired. A typical porous catalyst has a pore scale on the dimensions of nano-metres, and the catalyst itself may consist of particles ranging in size from microns to millimetres. The void space inside the reactor is also typically on the millimetre scale, and the reactor itself may have dimensions on the scale of metres. To solve the governing PDE for the reactor requires the spatial discretization of the solution domain, however, a complete discretization of all scales is either extremely time consuming or not possible at all. Usually only the largest scale is discretized and some form of volume averaging is used over the domain. The challenge is to incorporate the smaller scale information in the large scale model. This is usually done using sub-models, referred to generically as scale bridges. Scale bridges can be as simple as an algebraic equation or require the solution of a complex set of PDE on a sub-grid. The efficient choice of a scale bridge is often crucial to achieving a cost effective and timely solution.

This talk will discuss some methodologies for hierarchical multi-scale model reduction. It will focus on the use of pre-computed data stored in look-up tables as a means of achieving said computational efficiency. Some practical examples used in the modelling of structured reactors will be illustrated.

Biographical Notes:

Professor R.E. (Bob) Hayes is a Professor of Chemical Engineering at the University of Alberta. He has been active in Catalysis since his undergraduate years. Following a B. Eng. earned at the Technical University of Nova Scotia (TUNS), he pursued a PhD with Professor John Thomas at the University of Bath, UK. He continued his work on catalysis at TUNS as an Assistant Professor, studying the methanation reaction, before moving to the University of Alberta in 1985. Since 1990, he has worked in the area of catalytic combustion in structured catalytic reactors, both for the mitigation of fugitive methane emissions and in the development of automotive catalytic converters. The research work has been conducted in collaboration with both industrial and governmental laboratories, as well as with colleagues and other Canadian and International Universities. He is the author or co-author of

over 100 scientific papers and six textbooks, including the reference work, *Introduction to Catalytic Combustion*, published in 1997, and is co-author of the historical fiction novel *Riot and Retribution*.

His current research interests include catalyst development for the low temperature oxidation of methane in lean and wet gas streams, kinetic and reactor modelling of automotive exhaust gas after treatment systems and catalytic distillation for the production of biofuels.

Plenary Lecture #2

Chemical Engineering in Beer Making

Prof. Mario Jolicoeur and Mr. Philippe Leclerc
Department of Chemical Engineering, Polytechnique Montréal

This keynote lecture is an introduction to the wonderful world of beer making. Why beers have different colours? Why beers have different tasting profiles? These are the questions you will get answers to! From the history of beer to its final conditioning, this conference will guide you through the brewing process and how chemical engineers are there to optimize every step. A list of the key equipment you require to brew at home will be given and explained.

Biographical Notes

Philippe Leclerc

Philippe got his bachelor's degree in chemical engineering from Polytechnique Montreal in 2012. He was the director of "Polybroue", a technical society of brewing engineering and the director of "Les Houblonneries", a beer festival at Polytechnique Montréal. He is now conducting a Ph.D. in chemical engineering at Polytechnique Montreal under the supervision of Prof. Jamal Chaouki and Dr. Jocelyn Doucet. He has been an amateur brewer since 2006 and brewed over 100 beers. Over the years, he built a small home brewery using the chemical engineering knowledge he gathered during his curriculum.

Mario Jolicoeur

Mario Jolicoeur is a professor of chemical engineering at Polytechnique. He graduated in chemical engineering in 1987 at Polytechnique. He obtained a Master degree (Poly) in 1990 designing bioreactor for complex fluids, and then worked as a process engineer for four years and a half, in biotechnology. He then performed Ph.D. studies (1994-98), also at Polytechnique, but with multiple prolonged stay at the Université Paul Sabatier in Toulouse, France, followed by a postdoc at MIT on metabolic engineering. As an undergraduate student, he started making wine and has never stopped since. However, encouraged by Philippe and his co-brewers of Polybroue, he has set up a graduate course on beer brewing on the winter semester of 2013. Although he avoids thinking as a chemical engineer while making wine, he discovered that designing and making beers is an amazing playground for chemical engineers and especially for biochemical engineers.

Plenary Lecture #3

Intellectual Involvment merits Authorship Workshop

G.S. Patience, D.C. Boffito, P.A. Patience
Chemical Engineering, Polytechnique Montréal

The International Committee of Medical Journal Editors (ICMJE) states that individuals merit authorship when they participate in at least one activity from the following 4 categories:

1. Conception or design of the work; or acquiring, analyzing, or interpretation data; AND
2. Drafting manuscripts or revising them critically; AND
3. Approving the final version; AND
4. Agreeing to be accountable for all aspects of the work.

However, many articles in physics and medical categories attribute co-authorship to massive lists of researchers—some with 3100 individuals. In the humanities, law, and theology, writing constitutes the prime intellectual activity so articles are authored by one individual. National Institutes of Health (NIH) developed a scale for fifteen research activities. Together with ICMJE's fourth criteria, individuals might merit authorship when they contribute to one of the 15. However, supervision is underrepresented in their list–professors might not qualify as authors by the NIH.

This workshop addresses the question "What intellectual involvement merits authorship?" We identify research activities of 5 categories of scholarship–supervision, experimental design, sample manipulation, data reduction and writing.

Seminar Abstracts

Hicham Alayan

Title: Properties of bioplastics made from poly(hydroxyalkanoate) (PHA) resins

Supervisor: M. Maric and R. Leask

Biosourced polymer blends can be made from fermentation products of poly(hydroxybutyrate)-co-poly(hydroxyvalerate) (PHBV), crystalline poly(hydroxy-3-butyrate) (c-PHB) and amorphous poly(hydroxy-3-butyrate)-co-poly(hydroxy-4-butyrate) (a-PHB). The glass transition temperatures and mechanical properties of the polymers blended with primary and secondary plasticizers were characterized. The blends were plasticized using a green plasticizer, diheptyl succinate (DHPS), as a primary plasticizer, and epoxidized soy bean oil (ESBO) and stearic acid (SA) as secondary plasticizers. Blends with a-PHB were found to exhibit superior mechanical properties and lower glass transition temperatures compared to PHBV and c-PHB. A 49% increase in elongation at break in a-PHB has been achieved with the addition of 5 wt% ESBO and 1 wt% SA; however, the addition of DHPS was found to result in inferior mechanical properties of the blends, which can be attributed to potential phase separation. Ageing characteristics were also observed for the examined PHA resins as the blends were found to exhibit increasing crystallinity and decreasing elongation at break with time.

Ali Aljishi

Title: Ni-Ordered mesoporous catalyst for CO_2 methanation

Supervisor: J. Kopyscinski

Due to the intermittency of renewable energy sources, Power-to-Gas (P2G) concept is proposed in which electricity is stored as chemical energy (ie, H_2, CH_4). Methane is preferred as it can be used in existing gas infrastructure. Methane is produced via catalytic hydrogenation of captured CO_2. For this process a new Ordered Mesoporous Nickel Alumina (OMNA) catalyst was developed that exhibit a better performance compared to commercial available catalysts due to its unique properties such as organized and high mesoporous surface area. This work investigates the influence of the catalyst synthesis method on the catalyst properties and reactivity. Catalysts were characterized using BET, TPR, XRD, SEM, and ICP. Catalytic activity towards CO_2 hydrogenation was tested in a fixed bed reactor at different conditions.

Sara Babaei

Title: The effect of surface chemistry and protein adsorption on monocyte adhesion to plasma deposited functional organic coatings

Supervisor: P.L. Girard-Lauriault

Monocytes and macrophages play an initiating role in the foreign body response to biomaterial implants. The interactions between monocytes and biomaterials can potentially be modulated by controlling the surface chemistry and morphology of biomaterials. Organic coatings with varying oxygen and nitrogen concentration were prepared by low-pressure plasma co-polymerization of binary gas mixtures combining a hydrocarbon (C_2H_4 or C_4H_6) and a heteroatom-containing gas. (NH_3 or CO_2). The effect of surface chemistry on protein adsorption and on adhesion and differentiation of inflammatory cells to plasma polymer films containing tuneable concentrations of N and O functional groups were investigated. The study of protein adsorption by surface plasmon resonance results and the cell culture experiments revealed that the presence of albumin on the surface appears to act as an indicator for cell adhesion within the scope of our study.

Mitra Bahri (Concordia)

Title: Application of metal organic frameworks as dual functional adsorbent/catalysts for plasma air cleaners

Supervisors: F. Haghighat and D. Rohani

Over the past decade, plasma-catalyst systems have been considered as indoor air treatment methods for removal of volatile organic compounds (VOCs), particulate matter, and bacteria. It has been demonstrated that utilizing a dual functional adsorbent/catalyst (DFA/C) can significantly enhance the VOCs removal and the energy efficiency of such systems.

For the first time, this research attempted to utilize metal organic frameworks (MOFs) as DFA/Cs for a plasma-driven catalytic reactor. Accordingly, three different MOFs, MIL-101 (MIL: Material Institute Lavoisier), MIL-53, and CPM-5 (CPM: Crystalline Porous Material-5), were synthesized through microwave, solvothermal, and mechanochemical methods. To test the performance of these MOFs, a non-thermal plasma dielectric barrier discharge (DBD) system was designed, set-up and calibrated. Several adsorption and oxidation experiments were conducted to study the performance of these MOFs for the removal of toluene and isobutanol. Results demonstrated the high capacity of MIL-53 and MIL-101 as DFA/Cs in plasma-catalyst air purification system.

Christine Beaulieu

Title: Understanding granular segregation mechanisms in a horizontal drum: numerical study with DEM

Supervisors: F. Bertrand and J. Chaouki

Rotating drums are versatile equipment frequently used in industry, such as for drying operations in the mining industries, or for pyrolysis of solid wastes. However, despite their widespread popularity, their efficiency is often related to the homogeneity of the material inside the drum. Such particulate systems do not behave like fluids and one of their most striking characteristics is that they segregate. Granular segregation in rotating drum is quite well documented but not fully understood. In particular, some observed peculiar segregation patterns require further investigation to be able to predict precise granular flow dynamics and heat transfer inside a rotating reactor. To do so, we resort to both computer simulations and experiments. More precisely, models based on the discrete element method (DEM) are used to simulate the segregation of particles of different properties. Ultimately, the goal of our work is to assess the impact of granular segregation on the evolution of temperature in rotary kilns that are heated indirectly, as is commonly done in industry.

Ipsita Bordoloi

Title: Inhibition of carbon steel corrosion in closed-loop water-heating systems by using sodium caprylate as an environmentally-friendly corrosion inhibitor

Supervisor: S. Omanovic

In closed water systems water undergoes alternate heating and cooling by circulating in a closed cycle without exposure to air. Carbon steel finds wide application as material of construction for piping, boilers and radiators used for closed water systems. However, presence of dissolved oxygen, high salt content, variable temperature and pH cause internal corrosion and it is the main reason behind failure of closed water transporting systems. To mitigate this problem, corrosion inhibitors are widely used. However, due to health hazards related to commercial corrosion inhibitors, focus has shifted towards development of environment friendly corrosion inhibitors. The main objective of this work is to investigate the possibility of using sodium caprylate as an environment friendly organic corrosion inhibitor for carbon steel using various electrochemical techniques and surface analysis methods.

Anne-Marie Boulay

Title: The evolving concept of water scarcity and water footprint: when state-of-the-art and international consensus meet

Supervisor: M. Margni

As water has become one of the international priorities from government and NGOs, metrics to quantify its optimal use have become the center of attention. A water footprint is one such metric which assesses potential environmental impacts associated with water, at each step of the life cycle of a product (or service or organization). These concepts are now framed in a first international consensus on the principles, requirements and guidelines: the international standard ISO 14046:2014. At the core of this assessment, scarcity indexes are used to compare water consumption in different regions of the world facing different water situations. This paper presents the additional consensus work from the UNEP-SETAC Life Cycle Initiative working group on Water Use in LCA (WULCA), which achieved an internationally recommended method, called AWaRe, to apply the ISO standard and perform a water scarcity footprint.

David Brassard

Title: Heat dissipation in an electrically conductive nanocomposite

Supervisors: J.R. Tavares and M. Dubé

Adding electrically conductive nanoparticles to a polymer produces a nanocomposite which can be used as a resistive heat source. To efficiently use these nanocomposites, the mechanisms of heat generation must be understood. Finite element models (FEM) simulating heat generation inside a carbon nanotubes-reinforced poly(ether ether ketone) (MWCNT/PEEK) nanocomposite were developed. The models represents three possible sources of Joule heating: within the nanoparticles, at the contact resistance points and within the polymer. From the models, Joule heating of the MWCNT and contact resistance are the primary heating mechanisms. In addition, a homogeneous heating of the polymer, with negligible temperature gradients is observed. A MWCNT/PEEK wire was produced and heated under an electrical field to confirm the parameters of the FEM. The polymer reached a surface temperature of 190°C after 5 s. It is shown that MWCNT/PEEK nanocomposites are stable and reusable heating elements.

Madhuwanthi Buddhadasa

Title: N-rich plasma polymer films to regulate fibrinogen adsorption

Supervisors: P.L. Girard-Lauriault and S. Lerouge

N-rich plasma polymer films are deposited in a plasma enhanced chemical vapour deposition (PECVD) system using gas mixtures of ammonia/ethylene or ammonia/1,3-butadiene. These films, owing to their surface N functional groups, such as amines which are positively charged in aqueous media, can attract negatively charged biological molecules. We investigate the adsorption process of fibrinogen (Fg), a main blood protein that plays a vital role in blood coagulation, as a function of films' surface chemistry. The film chemical composition is determined by XPS and derivatisation with 4-trifluoromethylbenzaldehyde. Surface plasmon resonance spectroscopy is used to determine the thickness of the adsorbed Fg layer and adsorption kinetics. Dynamic contact angle measurements allow to study the role of wettability on the adsorption process. A strong dependence of adsorption kinetics on the film's surface chemistry is observed. Conformation of adsorbed proteins combined with possible adsorption mechanisms are discussed.

Marlon Bustos

Title: Effect of calcium carbonate on the mechanical properties of poly(hydroxyalkanoate) /green plasticizer blends

Supervisor: M. Maric

Poly(hydroxyalkanoates) (PHAs) are bio-based linear poly(esters) that have been considered as potential replacements for synthetic polymers in many applications traditionally using petroleum-based thermoplastics. However, PHAs exhibit thermal and mechanical properties that are not comparable to those of fossil-based polymers. To overcome these deficiencies, additives such as plasticizers, fillers, and heat stabilizers are used. In this study, several blends of an amorphous PHA with plasticizers and a filler were extruded. Diheptyl succinate and epoxidized soybean oil, both biodegradable plasticizers, were blended with calcium carbonate filler, which was appropriately surface treated to improve dispersion into the matrix. Additionaly, dicumyl peroxide has been added to the formulation to promote crosslinking of the polymer. Improvements up to 55% in the elongation at break due to the reactive extrusion with diheptyl succinate and calcium carbonate have been observed thus far in this research.

Francois-Johan Chassaing

Title: Development of a novel ozonation system for wastewater disinfection and removal of CECs

Supervisor: V. Yargeau

Contaminants of emerging concerns (CECs) are a source of concern as they are continuously released in receiving waters along with treated wastewater and have been shown to be detrimental to the aquatic environment. Ozone, known for its strong oxidizing properties, can be added to wastewater as a tertiary treatment to disinfect the wastewater and to tackle the CECs problem. The use of metal-based catalysts to increase the oxidizing power of ozone has been demonstrated in lab-scale studies, but efficiency had not been tested at a pilot scale. The objective of this thesis was to assess the effectiveness of selected catalysts using a continuous catalytic ozonation pilot scale system. Results showed that in presence of the most promising catalysts, the ozone requirement for disinfection was decreased, that an elevated removal of CECs was obtained using catalytic ozonation when compared to conventional ozonation, and that lower residual estrogenic activity was obtained.

Basant Elsiwi

Title: Diheptyl succinate (DHPS) – a really green plasticizer

Supervisors: M. Maric and R. Leask

The plasticizer di(2-ethylhexyl) phthalate (DEHP) is widely used to impart flexibility and malleability to polymers such as poly(vinyl chloride) (PVC). DEHP has the tendency to leach out of polymers and has been shown to biodegrade to toxic metabolites. These compounds have been linked to endocrine disruption as well as to a range of adverse effects in the liver, kidneys, lungs and heart. The ubiquitous presence of DEHP and its stable metabolites is of great concern. Earlier work at McGill has identified that succinate-based plasticizers are potential “greener” replacement plasticizers for DEHP, with better biodegradation characteristics and comparable plasticizer properties. However, previous work used succinic acid and alcohol derived from petroleum-based feedstock to synthesis the plasticizers. In this work, diheptyl succinate (DHPS) was synthesized from sustainable resources and its biodegradation and plasticizer properties were compared to other succinate-based plasticizers. Biodegradation with the common soil bacterium Rhodococcus rhodocrous showed a half-life of 1.3 days estimated using a first order, initial rate approximation. The metabolites that appeared after 1 day were the monoester, heptanol and heptanoic acid but they were completely removed after 13 days. Mechanical properties such as the glass transition temperature (Tg), tensile strength and rheological properties such as the storage and loss moduli were evaluated from blends of 29 wt.% DHPS into PVC. DHPS performed similarly to other succinate-based plasticizers in terms of biodegradation time and mechanical properties. It thus can be considered to be a completely ‘green’ plasticizer alternative to DEHP.

Hassana Elzein

Title: Combining optimization and consequential life cycle assessment to investigate energy storage systems

Supervisors: T. Dandres, A. Levasseur and R. Samson

Consequential life cycle assessment (LCA) is a methodology used to evaluate the environmental impacts of decisions and policies. With the advance of technology, it became harder to assess the smart systems on which we are relying extensively, using the traditional consequential approach. This is mainly due to the investigation of pre-set scenarios and to the lack of temporal variability inclusions in LCA which inaccurately reflect their operations. In this project, we develop an LCA approach to investigate time-dependent systems. We optimize the consequential LCA to evaluate the deployment of energy storage systems in the grids by assessing their realistic operation. The proposed methodology optimizes real-time power generation, while respecting the storage constraints, consumers' demand and local generators' specs. Comparing the environmental impacts of the optimized and historical grids highlight a reduction in greenhouse gas emissions up to 61 % when optimizing the generation and deploying a storage system.

Alexander Emmott

Title: Using transesophageal echocardiographic strain imaging to predict the biomechanical properties of ascending aortic aneurysms

Supervisors: R. Leask

Aneurysms of the ascending aorta are a serious disease requiring open heart surgery and replacement with a synthetic graft to manage the risk of aortic wall rupture or dissection. It is a massively invasive procedure and Cardiac Surgeons need better metrics to select patients for surgery. Here, we propose using pre-operative transesophageal echocardiography (TEE) strain imaging with parallel blood pressure measurements to estimate the mechanical state of the aortic wall. Results demonstrate that simple stiffness moduli derived from TEE imaging co-vary with ex vivo tensile biomechanical measurements, including apparent stiffness and energy loss. The TEE-derived indices are also predictive of the disruption of the histopathological tissue structure that defines the disease.

Yannick Essigan

Title: Epoxy methyl as bio-plasticizers

Supervisor: G.S. Patience

En raison de la récente augmentation des coûts de production du biodiesel et de la nécessité d'utiliser de manière respectueuse de l'environnement, des bio-plastifiants obtenus à partir d'huiles végétales ont été développés.Bio- Plastifiant sont essentiellement constitués d'huiles végétales époxydées (EVO) (Comme l'huile de soja riche en composer insaturée). Ces types de produits ont obtenu de bonnes propriétés plastifiant et sont facilement biodégradables par des agents microbiens.Le principal problème associé à ces produits réside dans leur contenu Esters méthyliques saturés. Cette fraction ne peut pas être époxydée et a une affinité très faible avec le Polymère, de façon à ce qu'il tende à migrer à la surface plastique donnant des propriétés non souhaitées à la surface finale des produits. Le but de ce travail est de trouver les meilleures conditions de réaction en termes de rendement en époxyde.

Teresita Rode Garcia

Title: Effect of the preparation process on the architecture and the physicochemical properties of PLA-PEG nanoparticles

Supervisor: X. Banquy

The physicochemical properties of nanoparticles determine their behavior in biological systems. Identifying manufacturing parameters that influence these properties would help to develop more efficient nanoparticles.

In this study, we compare the nanoparticles produced by Classic Nanoprecipitation, Flash Nanoprecipitation and Microfluidics in order to define the influence of the manufacturing process on the physicochemical properties. Also, for each method, three drugs with different Log P value were used to load the nanoparticles, in order to evaluate the join effect of Log P and fabrication method on the encapsulation efficiency.

We observed that the size, the polydispersity and the architecture of the nanoparticles were strongly affected by the fabrication process. On the other hand, the Zeta potential depended on the functional groups of the encapsulated drug. Also, we observed that the drug loading was not significantly affected by the fabrication method and the main property that determines it was the Log P.

Oscar Aguilar Gutierrez

Title: Flow induced alignment of dilute collagen solutions in mixed flows for plywood formation

Supervisor: A. Rey

Dilute isotropic collagen solutions are usually flow processed into monodomain chiral nematic thin films for obtaining highly ordered materials by a multistep process that starts with complex inhomogeneous flow kinematics. Here we present simulations with the response of such plywood precursors when submitted to the four roll mill kinematics where different types of flow can be simulated. We provide the kinematic conditions to which the collagen solutions should be submitted in order to produce a monodomain chiral nematic film.

Kieran Horry

Title: Bio-lubricant production using ultrasound and a heterogeneous catalyst

Supervisors: D. Boffito and F. Galli

Bio-lubricants are a possible alternative to their fossil-fuel derived counterparts; they are renewable, biodegradable and produce less toxins when combusted. Mass transfer limitations associated with their production may be reduced using ultrasound (US). Literature suggests US greatly increases the reaction rate by initiating hydrodynamic and acoustic cavitation, disrupting the phase boundary which encourages oil-alcohol emulsion formation. Separation issues can be minimised using a heterogeneous catalyst.

The reaction for study will be a catalysed esterification reaction forming a triester (bio-lubricant) and water from trimethylolpropane (TMP) and oleic acid. The reaction will be catalysed by a heterogeneous acidic catalyst, namely phosphotungstic acid on an aluminium oxide support. The effect of US on the reaction rate will be examined, as well as US pulsation. Alternative catalysts and reaction temperatures may also be tested.

It is predicted that US will greatly increase the oleic acid consumption rate and improve bio-lubricant yield.

Adya Karthikeyan

Title: Carbon nanotube nanofluid-metal interaction

Supervisors: S. Coulombe and A. Kietzig

Nanofluids are colloidal dispersions of nanoparticles in base liquids. They captivate the interests of researchers and technologists since their introduction in the literature in the late 1990's. A rich literature reports that the heat transfer properties of nanofluids vary from those of the base liquids. However, there is no consistency in the results and many controversies exist. It has recently been established that the instability of nanofluids contributes to the contradictions reported. In addition, we put forth that for nanofluids to be used for heat transfer applications, they should remain stable when they are in contact with metals. In this work, we used nanofluids made up of oxygen-functionalized multiwall carbon nanotube (F-MWCNT) in ethanol, water, and ethylene glycol which remain stable when heated and when stored in glass vials. However, we observed that only the ethanol-based nanofluid remains stable in the presence of metal coupons. We report the reason for exceptional stability of ethanol nanofluid is the strong hydrogen bonding between the carboxylic groups on the F-MWCNT and the ethanol molecules. We investigated this using different techniques as particle size analysis, NMR, FTIR spectroscopy.

Evelyne Kasparek

Title: Fabrication and characterization of photo- and plasma-chemically deposited sulfur rich thin films

Supervisors: P.L. Girard-Lauriault, M. Wertheimer, and J.R. Tavares

Surface modification methods can be used to improve the performance of synthetic polymers. Some of these are based on "cold" plasma-based thin film deposition, in which electrons, ions and photons interact with a reactive gas to form a functional coating on the desired substrate. The resulting changes in surface composition, surface energy, and morphology can improve properties such as wettability, biocompatibility, etc.

Thin organic films incorporating sulfur-bearing functional groups have been prepared by "co-polymerizing" gas mixtures consisting of a hydrocarbon source, with H2S. This has been accomplished by either plasma-assisted chemical vapor deposition; or by vacuum-ultraviolet irradiation of the gas mixtures with near-monochromatic radiation from different lamps (λ=112-254 nm). Different VUV lamps have been used to investigate the wavelength dependency of the chemistry and stability of the films. All deposits were characterized by XPS before and after chemical derivatization with N-ethylmaleimide, which serves to quantify the thiol concentrations on the surfaces.

Ahmad Khan

Title: Ice and Hydrate Adhesion on Poly(N-vinylcaprolactam) Surfaces

Supervisor: P. Servio and M. Maric

The natural formation of hydrates in pipelines, due to high pressure and low temperature, results in plugging which leads to production hindrance. The oil and gas industry currently utilizes kinetic inhibitors to prevent hydrate growth, which results in over $200 M USD spent annually. An alternative to this form of hydrate inhibition is the use of surfaces which prevent clumps of gas and ice particles coming together to form hydrates. Poly(N-vinylcaprolactam), a polymer previously used as a kinetic inhibitor, has the potential to act as an enclosing material which inhibits the thermodynamically favored formation of hydrates on surfaces. The polymer was tested for hydrate inhibition by measuring the amount of force required to dislodge hydrates. If found to be inhibiting hydrate nucleation and subsequent growth, the oil and gas industry could potentially reduce their operational costs many times over for the price of integrating this approach in their pipeline infrastructure.

Liji Le

Title: Numerical calculation of gel electrophoretic mobility for “soft” spherical nanoparticles

Supervisor: R. Hill

Gel electrophoresis is conventionally used for sorting and separating macromolecules. More recently it has been adopted for nanoparticle sorting and characterization. While the theoretical interpretation of free-solution (without gel) nanoparticle electrophoresis is well developed, models for interpreting nanoparticle gel electrophoresis are new. Hill (2016) recently developed a generalized electrokinetic model that accounts for polarization and relaxation effects to calculate the gel electrophoretic mobility of functionalized/soft spherical nanoparticles translating in charged and uncharged gels. The model captures hydrodynamic effects based on the Brinkman approximation for particles with arbitrary size, and included pH charge regulation models. In this study, the model has been applied to compare with independent calculations in the literature (including those undertaken using commercial finite-element software). Theoretical interpretations of experimental gel-electrophoresis data for soft nanoparticles are presently in progress. To date, the model has accurately reproduced calculations in the literature, and extended the parameter space, now showing potential for quantitatively interpreting nanoparticle characterization and separation processes.

Philippe Leclerc

Title: Production of renewable styrene using catalytic microwave depolymerisation

Supervisors: J. Chaouki and J. Doucet

Polystyrene global demand is expected to reach 23.5 million tons by 2020, an increase of 57% compared to 2010. Yet, it is one of the less recycled plastic: a mass fraction of 1.3% of the generated polystyrene was recovered in the United Stated in 2013. Microwave pyrolysis can recycle polystyrene by breaking it down into styrene monomers. It can then be re-introduced in the existing ecosystem of refining and polymerization industries. However, microwave heating is known to induce changes in the reaction kinetic. These changes will be explained by looking at the dielectric properties of the polystyrene. They were investigated as a function of temperature and molecular weight. The results show that the dielectric properties of the polymer material change as a function of both the temperature and the molecular weight and that the dielectric loss tangent can vary up to a factor 20.

Wontae Lee

Title: Dispersible hydrogel mechanosensors to measure cell-generated stress within 3D cultures

Supervisors: C. Moraes and R. Leask

Within 3D tissues, cells exert local and directional forces that feed back to direct tissue shape and function. While it is recognized that cell-generated forces are critical in the biological lifecycle of multicellular organisms, measuring these forces in physiologically realistic microenvironments remains a challenge. We developed soft and compressible fluorescent hydrogel microdroplets that deform under cell-generated forces, enabling read-time and absolute read-outs of cell forces.

Microgels were embedded within fibroblast-laden contractile collagen gels; anisotropic forces were measured over 3 days of remodelling and following application of inhibitors and activators of cell contractile forces, demonstrating the real-time potential of the sensors. Microgels were embedded within fibroblast spheroids; spatial variations in forces were measured, demonstrating heterogeneity in simple spheroid cultures.

The sensors developed enable the real-time measure of local and absolute cell forces in 3D tissues, and may hence be used to address a broad range of fundamental and applied biological questions.

He Li

Title: Ultrasound assisted wet stirred media mill of high concentration LiFePO4 and catalysts

Supervisor: G.S. Patience

Micronization techniques grind solids to nanometric size; but water loading time and energy are critical factors that limit the commercial application. Ultrasonic and micronization coupling, increases the temperature of the medium, which will decrease the viscosity and facilitate the contact between solids. Ultrasound assistance increases the suspension solid loading capability during wet media milling. Acoustic cavitation generates extreme local temperatures and pressures (5000 K, 1000 bar), helping in the grinding process. LiFePO4 (LFP) suspension is shear-thinning: the instense shear force decreases the fluid viscosity and allowed us to increase the solid loading limit from about 45% to

60 %. When working with suspensions of LiFePO4 (LFP) when using: yttria stabilized zirconia media (YSZ) size from 0:3mm to 0:4 mm, surfactant-to-LFP mass ratio 0:008, and mill rotation rate 50 Hz, with 40% amplitude of 500W 20 kHz ultrasound assisting, we ground particle size from 35 µm down to 0:2 µm in 90 min with throughput at 0.68 kgLFP/kgmedia/h. The experimental data are in good agreement with the predicted data by model (R2 >0.95). We represent the steady state and repeat-able micronizing process with ultrasonic assistance. TEM imaging illustrated that the primary particles (20 nm) are much smaller than the agglomerated ones determined by laser diffraction.We developed and updated the steady state and repeatable micronizing process with ultrasonic assistance using a simplied population balance model. The experimental data are in good agreement with the predicted data by model (R2 > 0:95).

Paul Louyot

Title: Ultrasound process for Fischer-Tropsch iron catalyst synthesis
Supervisor: D.C. Boffito

Natural gas flaring and venting from oil wells are a major environmental concern. An alternative to flaring is to convert the gas into hydrocarbons with a mobile Gas-To-Liquids unit. We patented a double stage reactor housed in a single pressure vessel that first produces synthesis gas by catalytic partial oxidation, followed by Fischer-Tropsch at 300°C.

The latter reaction generally relies on supported iron or cobalt catalysts. Iron catalysts are less expensive but less active, and iron loading on the support surpass 15 %. This requires lengthy deposition steps and generates uneven dispersion.

We propose a method for the synthesis of supported iron catalysts by ultrasonic-assisted incipient wetness. We sonicate Al_2O_3 as a support in presence of metal nitrates with ultrasound pulses. This generates hot spots that are expected to ease metal ions adsorption on the catalyst support and improve the dispersion, thus accelerating the synthesis of the catalyst.

Zhenni Ma

Title: FeCralloy® partially oxidizes methane to syngas selectively

Supervisor: G.S. Patience

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 knitted fiber resists high temperatures, are highly conductive, and can be molded into shapes. It partially oxidizes methane to produce syngas. We improved its reactivity by dispersing Pt, Rh or CeO_2 over its surface via solution combustion synthesis. FeCralloy catalysts selectivity oxidize methane to syngas at 900^{o}C and from 0.1 MPa and 2 MPa; all the oxygen was consumed for all experiments, which is critical for the FT step that requires a reduced catalyst.

Mohammad Jaber Darabi Mahboub

Title: Transient methacrylic acid selectivity study with calcination temperature; correlation of catalyst structure and reaction mechanism

Supervisor: G.S. Patience

Methacrylic acid (MAA) is a specialty chemical that esterifies to methyl methacrylate (MMA), which is a monomer for poly-methyl-methacrylate (PMMA). Current processes partially oxidize olefins to MAA but require multipe steps and catalyst stability remains problematic. Partial oxidizing of 2-methyl-1,3-propanediol (2MPDO) to MAA over Keggin-type heteropoly compounds is a novel route. Here, we synthesize heteropoly catalysts, characterize surface and bulk properties, and measure selectivity during 8 h of activation. Calcining at higher temperature increases the interaction between vanadium and the Keggin-structure (stronger V2O5) which forms additional active site vacancies. The oxidation state of catalyst calcined at 350 C was higher than those calcined at 300 C but during reaction more of the Mo^{6+} reduced to Mo^{5+}. The higher extent of reduction confims the higher redox reaction between (Cs^{+} and NH^{+4}) and PMO12O40 (3-) beside, higher O^{2-} --- Mo^{6+} charge-transfer in the Keggin anion.

Maximum MAA and MAC selectivities were 61% and 28%, respectively at 250^{o}C

after 480 min over cycling oxidationreduction and 2MPDO/O2/Ar= 13/10/77 as the best reaction condition and feed composition.

Oscar Marin

Title: Phase equilibrium and liquid mole fraction measurements of tetra-n-butylammonium chloride + CO_2/CH_4 semi-clathrates

Supervisor: P. Servio

Clathrates hydrates have industrial applications in gas storage, transportation. They generally require high pressure and low temperature to form. A low-cost alternative exists which uses thermodynamic promoters such as tetra-n-butylammonium chloride. This promoter reduce the conditions of the hydrate equilibrium, allowing higher temperatures and lower pressures to form hydrates. This study reports phase equilibrium and liquid mole fraction measurement of TBAC + methane and TBAC + carbon dioxide semiclathrates. This is the first study to report the liquid mole fraction at equilibrium under three-phase hydrate-liquid-gas in the presence of the ionic salt TBAC. The importance of these measurements is liquid phase composition for reactor design and kinetic models. TBAC mass fraction of 5, 10 and 15 % were employed. Pressure from 0.8 to 4.7 MPa and 0.1 to 2.4 MPa; temperature from 280 to 290 K and 283 to 288 K for CH4 and CO2 respectively.

Meghan Marshall

Title: LuminoTox: A tool to monitor contaminants of emerging concern in secondary effluents and to evaluate their toxicity removal during ozonation

Supervisor: V. Yargeau

There is a need for more sensitive and rapid technologies to monitor contaminants of emerging concern (CECs) in wastewater and to minimize their associated toxicity. The LuminoTox and ozonation were evaluated for their ability to monitor and remove CEC toxicity, respectively. In most cases, secondary effluent characteristics did not interfere with LuminoTox toxicity measurements, suggesting that the bioassay would be applicable for the monitoring of such complex matrices. The LuminoTox was also shown to detect CECs with different modes of action while being more sensitive to CECs acting directly on photosynthesis, specifically on the plastoquinone binding site within photosystem II. However, LuminoTox was not able to detect CECs at environmentally relevant concentrations and a pre-concentration method was developed to increase its sensitivity. Finally, the mode of addition of a same dose of ozone to wastewater was shown to influence the removal of toxicity during treatment.

Luke Matus

Title: Laser chopper for downstream frequency reduction and pulse selection

Supervisor: A. Kietzig

Investigating the effect of different laser pulse overlap methods on surface damage requires reliable laser pulse selection. A 1 kHz Gaussian laser with a 5 mm 1/e2 beam width requires a shutter speed > 10 mm/ms which is unattainable by mechanical shutters with movement speed of about 1 mm/ms. Instead, we fabricated a downstream beam chopping device to pass 1 in 40 pulses reducing the laser frequency to 25 Hz. The device consists of an acrylic disk with an aperture rotated at 1500 RPM by a brush-less DC motor. The motor is driven by an Arduino Mega which locks to the laser frequency. Serial communication with a second Arduino allows user selection of pulses via a mechanical shutter placed in series with the chopper. With this technique, we were able to characterize the differences between damage features on moving and stationary surfaces.

Stephanie Mok

Title: Measuring local 3D tissue stiffness using microengineered smart material probes

Supervisor: C. Moraes

Changes in the mechanical properties of tissues are related to health and disease, but monitoring real-time changes of stiffness in-situ remain challenging. Current techniques are capable of bulk and local measurements of stiffness, but require specialized equipment and are limited to end-point analyses. Furthermore, they are restricted in their ability to spatially resolve cellular-scale stiffness variations in 3D tissues, which would be critical to characterize the stiffness a cell would experience in-situ. We have developed optically-measureable and dispersible cell-sized sensors that actuate by temperature control to exert a small local force within 3D tissue. N-isopropylacrylamide hydrogel beads demonstrate reversible size changes at a critical temperature just below body temperature. When embedded in soft materials, expansion is large, but is constrained when embedded in stiff materials. By measuring the size change in these sensors, local tissue stiffness can be extrapolated. This technique is easy to implement, inexpensive, amenable to high throughput analyses, and non-destructive to cells and tissues.

Emmanuel Nwanebu

Title: Development of NiCo-oxide anodes for oxygen evolution in electrochemical hydrogen production by water electrolysis

Supervisor: S. Omanovic

Hydrogen gas is regarded as the future energy fuel vector. Unfortunately, water electrolysis, the most environmentally viable hydrogen production option, is not energy efficient and requires expensive metals as electrodes. In the case of polymer-electrolyte-membrane (PEM) based electrolysers, both electrodes (anode/cathode) have to be noble due to the electrolysers' very aggressive acidic environment. Furthermore, the oxygen evolution side (anode) presents the major kinetics obstacle in water electrolysis. The current state-of-the-art anode is the Ir-oxide anode. However, iridium is very expensive, and in order to commercialize the PEM technology, iridium has to be replaced by a cheaper alternative, that yields satisfactory electrocatalytic activity.

This PhD project objective is to develop novel mixed-metal oxide anode materials (via thermal decomposition) with high electrocatalytic activity in oxygen evolution and good electrochemical and structural stability. The current talk will present our recent results on the development of NiCo-oxide as a potential replacement of Ir-oxide anodes.

Francois-Julien Pelletier

Title: Plasma-polymer coating reduces tetrahydrofuran hydrate adhesion

Supervisors: P. Servio and P.L. Girard-Lauriault

Natural gas pipelines are subject to plugging by the formation of gas hydrates due at high pressure and low temperature conditions. This study designs coating making the pipeline hydrate-phobic thus avoiding its plugging. For practical reasons (mass transfer and thermodynamics), tetrahydrofuran is used to form hydrates in this study. Metal substrates are coated with plasma polymer with the aid of a plasma-enhanced chemical vapor deposition (PECVD). The plasma polymers are composed of one carbon source (ethylene and butadiene) and one or more heteroatom (C, O, S and N). The sulfur-rich surface (butadiene + S) yielded the lowest adhesion strength with a value of 48%±14% of the baseline value. In this case, the plasma polymer was measured to be composed of approximately 1at.% sulfur with the balance being carbon. This study highlights the prime importance of chemical composition in hydrate adhesion since plasma polymer coatings show almost no surface topography.

Marco Giulio Rigamonti

Title: Spray dried VPP: core-shell morphology and attrition resistance

Supervisor: G.S. Patience

Imparting attrition resistance to fluidized bed catalysts is a critical factor to achieve an economic advantage over fixed bed technology. Here we spray dry vanadium pyrophosphate to form an attrition resistant core with a hard silica shell. Catalytic fluidized beds require spherical particles with a broad distribution (PSD) centered around 70 µm. Spray drying conditions, slurry rheology and precursor powder properties affect the particle morphology–density, shape, porosity and PSD. A wet media mill charged with yittria stabilized zirconia beads reduced the particle size of the precursor to 0.5 µm. Water suspended the solution with a combination of colloidal silica, polyvinyl alcohol and H3PO4 binders. A two-fluid nozzle atomized the slurry into a 0.9 m chamber operating at 250 ºC. EDS elemental mapping images of the powder demonstrated that the Si migrated to the surface during the drying process and forms a resistance shell.

Pardis Rofouie

Title: Surface Pattern Formation in Plant-based Plywoods and Biological Liquid Crystal Membranes

Supervisor: D. Pasini and A. Rey

Understanding the mechanisms through which living systems exhibit unique surface undulations and specific morphologies can inspire design and fabrication of bio-inspired structural and functional materials. This work explores the physics of wrinkling formation in cholesteric liquid crystal interfaces as the representative analogues in plant cell wall and nematic liquid crystal closed membranes as the representative analogues in living cell membranes. A comprehensive physical model using anisotropic soft matter models is developed to create new knowledge and principles for studying the role of liquid crystal anisotropy in the formation of surface morphologies. By taking advantage of geometry and system material constraints, the key physical parameters that affect the formation of the surface morphologies are identified. Comprehensive phase diagrams of morphological surface patterns are illustrated that enable us to predict the surface patterns and membrane shapes depending on the system physical parameters. Moreover, potential biomimetic application of the surface ultrastructures is demonstrated.

Hajer Rokbani

Title: Rheological properties of the Poly(D,L-Lactide) solutions added with metal oxide nanoparticles.

Supervisor: A. Ajji

PLA nanocomposites with antibacterial properties are of great potential interest as food packaging biomaterials. The investigations carried out in this study include the rheological properties of PLA/ZnO nanoparticles solutions used for electrospinning of nanofibrous mats as well as the morphological evaluation of the mats thus obtained. The effect of ZnO nanoparticles was investigated for various PLA solutions and solvents. The PLA solutions with low loading level of ZnO nanoparticles showed higher viscosity (μ) than the neat PLA. They also showed a maximum value of μ at 3 wt % content. Solutions containing more than 3 wt % ZnO exhibited a notable decrease in viscosity, which could be due to PLA degradation. Whereas in the case of others nanoparticles like SiO_2 and TiO_2, no decrease in the solution viscosity was recorded.

Nooshin Saadatkhah

Title: Flame-assisted spray pyrolysis (FASP) hollow shell C-$LiMn_2O_4$ from aqueous solution

Supervisor: G.S. Patience

Particles properties of a cathode strongly controlled electrochemical properties of the cathode; particles properties such as morphology, specific surface area, crystallinity, and composition. $LiMn_2O_4$ (LMO), one of the alternatives for Li_2CoO_2, with three-dimensional octahedral structure and intersecting tunnels allow for three-dimensional diffusion of lithium ions.

We synthesized Spinel $LiMn_2O_4$/ hollow shell powders by a flame-assisted spray technology (FAST). The precursor is an aqueous solution consists of $LiNO_3$ and $Mn(NO_3)_2$.xH2O or Li2CO3 and $Mn(CH_3CO_2)_2$.4H2O in stoichiometric. The as-synthesized $LiMn_2O_4$ particles were nano-crystalline with impurity of Mn_3O_4.

Nano particles increase surface area, diffusion rate and capacity. Carbon network increase intra-particle conductivity and increase available capacity. While products from carbonaceous precursors has a minimum of 2 % carbon content, nitrate precursors produce products with 0.1 % carbon content.

Amin Sadeghi

Title: The interplay between pore structure and electrode performance: a pore network modeling study

Supervisor: J. Gostick and P. Servio

With the advent of large scale harvesting of renewable energies, developing high capacity energy storage systems is necessary. This necessity is largely due to the mismatch between the energy generation and consumption peaks. Flow batteries are a promising technology to be used as part of such large-scale energy storage systems. The flow battery is similar to a conventional battery except that the active materials is no longer the solid electrode, but a flowing liquid electrolyte that reacts at the liquid-solid interface. This decoupling allows for easier upscaling of storage by simply increasing the size of the liquid reservoirs. Optimizing the porous structure of the electrodes of a flow battery is a possible way to maximize its performance and lowering cost. In this study, pore network modeling was used to study the effect of the electrode pore structure on the performance of a flow battery. Unlike continuum volume-averaged models, pore network modeling explicitly accounts for the microstructure of porous materials.

Ali Sahmoud

Title: McGill Chem-E Car Design Team

Supervisor: C. Moraes

The McGill Chem-E Car Design Team competes at the AIChE nationals and regionals competitions. The teams are required to design and build shoebox sized cars powered and stopped by chemical reactions. The car should safely transport a specified load of water over a given distance, both values are unknown until one hour of the competition. The power source for the car is a soluble lead flow battery that requires the usage of only one electrolyte and does not require any membranes. The stopping mechanism is the Iodine Clock reaction which changes color instantaneously from colorless to black, this change is detected by a light sensor developed by the team that cuts the current from the motor containing a spur gear, thus stopping the car at the required distance. The team also designed a stirring mechanism to increase precision and accuracy.

Sanya Siddiqui

Title: The development of an in vitro co-culture device for bacterial infection studies

Supervisors: C. Moraes and N. Tufenkji

Engineered co-culture systems enable controlled cell-cell interaction studies that would not be possible using petri dish cultures or animal models. However, the complex interactions between bacteria and mammalian cells are challenging to recreate using existing technologies. Long-term co-culture to study the progression of infection is especially difficult as the overgrowth of bacteria and their secreted by-products cause excessive death of the host cells. Compartmentalized microfluidic platforms can be used to improve current co-culture platforms as they allow effective control over communication between microscale chambers, while replicating features of the tissue microenvironment. In my research, a bacterial infection-on-a-chip device was designed, built and tested. Bacterial and mammalian cells were cultured in the device to mimic infection and tested to study long-term interactions between the two cultures. This platform can be applied to study various bacterial infections and aid in identifying new strategies for the diagnosis, treatment and prevention of bacterial infections.

Kanayah Thumiah & Mohamad Kabbara

Title: Conception et analyse d'impact d'une usine de prétraitement de catalyseurs usés

Supervisor: J.R. Tavares

Les catalyseurs usés provenant des unités pétrochimiques sont un déchet important pour cette industrie. (Marafi, & Stanislaus, 2003). Plus encore, avec des règlementations environnementales de plus en plus strictes, il est important d'envisager des alternatives à l'enfouissement traditionnel. (Hatch, 2016). Ainsi, Hatch Ltée mandate la conception et l'analyse d'impact d'un procédé qui permettra la récupération des hydrocarbures résiduels et le décokage des catalyseurs usés en Alberta, Canada. Et ce, dans le but d'acheminer ce catalyseur prétraité pour des prochaines étapes de valorisation des métaux.

Ray Tran

Title: A biomimetic approach to study the role of tissue shape on pancreatic stem cell differentiation

Supervisors: C. Hoesli and C. Moraes

Production of insulin-producing beta cells from induced pluripotent stem cells (iPSCs) is a promising, sustainable avenue to replace native cells destroyed by type 1 diabetes. However, current protocols are inefficient and produce immature cells. These protocols do not capture biophysical forces and geometric cues present during embryonic development which are hypothesized to aid pancreatic differentiation. To investigate, novel cell culture systems to induce cellular tension were fabricated and tested with iPSC-derived pancreatic progenitor cells. The ~80% PDX1-positive pancreatic progenitor cell population was obtained from published pancreatic differentiation protocols. Agarose microwells were fabricated to spatially confine cells during differentiation. To mimic developmental geometry, curved microchannels were fabricated using microfabrication techniques. Pancreatic progenitor cells cultured within these devices were viable. Preliminary results suggest microwells alter aggregation and differentiation dynamics. These results provide a basis to investigate the effect of tension in pancreatic embryonic development and to design improved pancreatic cell production systems.

Michael Wood

Title: Development of a millimetric droplet generating apparatus

Supervisor: A. Kietzig

High-speed drop impact tests have emerged in recent years alongside developments in high-speed imaging which attempt to reproduce real-world surface wetting scenarios in the lab environment. The success of high-speed drop impact testing rests heavily on the ability to reliably produce millimetric liquid droplets. A novel water droplet generating apparatus has been developed to ensure that droplets produced are of a well-defined volume. This is achieved by the employment of a tee-apparatus, which serves to separate the desired droplet volume from the bulk liquid supply in a step prior to the discharge of the droplet. Further, the apparatus was designed to produce droplets which have minimal oscillation in their volume and follow a well-defined trajectory throughout their descent. These characteristics are achieved by manufacturing a superhydrophobic generating tip through femtosecond laser micromachining. Thus, a weakened solid-liquid interaction is exhibited at the point of droplet discharge.

Shengnan Yan

Title: Effect of particle pore size on RTD

Supervisor: G.S. Patience

Residence time refers to the time the material flowing through an equipment. It is widely used across all engineering disciplines, including chemical engineering, biological systems engineering, biomedical engineering, civil engineering, environmental engineering and geological engineering. Chemical engineers use the residence time distribution (RTD) to characterize the mixing and flow within reactors and to compare the behavior of real reactors to their idea models. This is very meaningful, not only for troubleshooting existing reactors, but in estimating the yield of a given reaction and designing future reactors. Few researches have been done about the effect of particle pore size on gas phase RTD in a fluidized bed. My future work is mainly on this point.

Nariman Yousefi

Title: Hierarchically porous graphene oxide-cellulose nanocrystal sponge for water treatment

Supervisors: N. Tufenkji

Three dimensional graphene-based sponges have been widely used as efficient sorbents for contaminant removal from water and wastewater. The self-assembly of graphene oxide (GO) into 3D architectures such as sponges usually results in their restacking, which reduces the effective available surface area of the sponges, and also results in decrease in their mechanical properties. In addition, poor distribution of GO nanosheets in sponges leads to formation of isolated pores with poor interconnectivity. In this work, we use vitamin C and 1D cellulose nanocrytals for processing nanohybrid GO-based sponges with a unique bimodal hierarchical pore architecture. The pore structure of sponges is characterized by high resolution scanning electron microscopy and micro- and nano X-ray computerized tomography (CT). With the aid of micro- and nanoCT 3D reconstruction of the sponges, the pore structure, porosity and the surface area parameters are calculated for a relatively large volume of the sponge. The highly porous sponges are shown to adsorb a wide variety of contaminants from aqueous solutions.