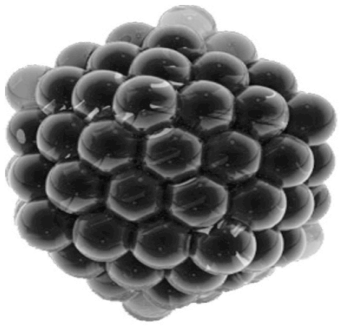

UPRM-Chemical Engineering Graduate Research Symposium

Friday, May 3rd, 2013 – Celis 116 & Salón Tarzán (Cafeteria Annex)

Sponsor:

P&G

Coordinator: Prof. Ubaldo M. Córdova-Figueroa

Agenda

Activity / Seminar Title	Speaker	Time
Registration & Breakfast (Cafeteria Annex)		7:30-8:40AM
Welcome (at Celis 116)		8:40-8:50AM
Synthesis of a novel polyether block copolymers for fuel cells and specialty separations applications	Maritza Perez	8:50-9:20AM
Synthesis of mesoporous carbon catalytic materials with improved thermo solvent stability for dehydration reactions of biomass-derived feedstocks	Christian Rivera	9:20-9:50AM
Catalytic Conversion of CO_2 to hydrocarbons	Oscar Oyola	9:50-10:20AM
Break		10:20-10:30AM
Keynote: A comprehensive approach to cancer treatment using magnetic nanoparticles: from basic engineering to in vivo studies	Prof. Madeline Torres	10:30-11:30AM
Lunch, Poster Session (at Cafeteria Annex)		11:30AM-2:00PM
Rheology of hard-sphere and square-well suspensions by Brownian dynamics simulation	Ronal De La Cruz	2:00-2:30PM
The effect of particles with asymmetric friction coefficient to the flowability of granular materials	Efrain Aymat	2:30-3:00PM
Continuous tumble mixer characterization	Miguel Florian	3:00-3:30PM
Awards, Closing Remarks & Evaluation		3:30-4:00PM

Poster Presenters	Title
Carlos Pinzón	Flavoring Effect on the Thermal Gelation of HPMC Physical Gels
Ariangelís Ortiz	Analysis of the effect of the addition of titanium dioxide to sulfonated poly(styrene-ethylene/butylene-styrene) (SEBS) membranes
Angelica Roman	Polymeric Nanocarriers as Vehicles for the Treatment of Lysosomal Storage Diseases
Ana Cameron	Rheology of Rod-like Nanoparticles in Liquid Crystal Polymer Solutions
Wilma Cabrera	Adsorptive Removal of Carbamazepine and Salicylic Acid from Water Using a Zeolite Modified with Extraframework Transition Metal Cations and a Surfactant
Meghan Clardy	Development of Iron Oxide Nanoparticles with Enhanced Energy Dissipation for Application in Magnetic Fluid Hyperthermia
Stephany Herrera	Synthesis and Characterization of a Polysiloxane Based Liquid Crystalline Elastomer

Keynote Speaker: Prof. Madeline Torres

Title: A comprehensive approach to cancer treatment using magnetic nanoparticles: from basic engineering to in vivo studies

Abstract: The use of magnetic nanoparticles for biomedical applications, in particular cancer treatment, has been investigated for more than a decade. In vivo temporal and spatial control are still challenges that must be faced in order to make the clinical application of these systems a reality. Our work has focused on the in depth understanding of the nanoparticle's surface properties and the resulting in vitro and in vivo behavior. This presentation will summarize lessons learned and the contributions of our work in this area.

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral ( ) Poster (*)

Polymeric Nanocarriers as Vehicles for the Treatment of Lysosomal Storage Diseases

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Department of Chemical Engineering, University of Puerto Rico-Mayagüez

ABSTRACT: Lysosomal Storage Diseases (LSDs) are a group of inheritable genetic diseases caused by mutant lysosomal enzymes, leading to the accumulation of undigested macromolecules in the lysosomes and causing increases in lysosome size and number, cellular dysfunction, clinical abnormalities, and premature death. These LSDs can be treated with Enzyme Replacement Therapy (ERT) through intravenous administration of a recombinant enzyme in replacement of the defective enzyme. However, this is an expensive and inefficient method with adverse side effects associated with the high enzyme amounts required for the treatment, the need of post-translational modification of the enzyme and the host immune system response.

We hypothesize that nanocarriers composed of Polyethylene glycol and Polycaprolactone (PEG-PCL) block copolymers can enhance ERT by eliminating the need of enzyme modification and protecting it from host immune system until lysosomal target is reached. We have designed these nanocarriers to remain stable at physiological pH and destabilize at acidic pH, making them reach the cell intact and degrade once inside the acidic lysosome, therefore releasing therapeutic cargo into affected cellular organelle.

In order to obtain the appropriate nanocarriers for ERT application, we synthesized a group of PEG-PCL nanocarriers, varying the production process and surfactant concentration. The most suitable combination was found by performing dynamic light scattering analysis (DLS), gel permeation chromatography (GPC), Themogravimetric Analysis (TGA) and several spectroscopic techniques. We found the nanocarriers are not cytotoxic in cell lines tested. We are currently working on the reproducibility of syntheses and protein loading capacity into nanocarriers.

Keywords: Nanocarriers, PEG-PCL, LSD, ETR

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral (x) Poster ( )

Continuous Tumble Mixer Characterization

Miguel Florian, Rafael Mendez
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Seventy Percent of the global pharmaceutical production includes tablets manufacturing in which the mixing is an essential operation. Currently, mixing is performed in batch mode with several problems and limitations; two of the main problems are how to determine uniformity and the limitation to apply control strategies. The FDA and the pharmaceutical companies are proposing the use of continuous process as a solution. This investigation work includes the characterization of a new continuous tumble mixer to study granular mixing.

This study focuses on the effect of material properties, API concentration (2.5, 10.5 and 20%), and equipment parameters (including RPM, flow rate, and feeding angle) on the powder behavior and on the final blend uniformity. Based on the experimental results a simulation set was performed using Discrete Element Methods to study cohesion effect, velocity profile, particle trajectory, and powder phenomena inside the mixer. An experimental set with the same operational parameters was run to validate the simulations. The principal results showed RSD values below 6% for the experimental part and below 3% for the simulations; and that the cohesion, speed mixer, flow rate and feeding angle affect the final uniformity.

Future works include the effect of particle size, density, filling ratio and scale-up process on the final blend uniformity.

Keywords: Continuous Mixing, Tumble Mixer, DEM Simulation.

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral (x) Poster ( )

Catalytic Conversion of CO_2 to hydrocarbons

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ABSTRACT: Carbon dioxide is the most abundant greenhouse gas. One option to mitigate its emissions involves its catalytic conversion to useful compounds especially fuels. In this regard, we are working with Pd-GaO_3 supported on silica, Cu-ZnO supported on silica and GaO_3 catalysts to produce methanol and dimethyl ether via CO_2 hydrogenation. We are currently studyin the catalytic performance of these materials using a fixed bed flow reactor system. The Cu-Zn/SiO_2 catalyst presents 100% selectivity to methanol, but has low yield compared with Pd-GaO_3/SiO_2. Also the effect of surface area on selectivity and yield is studied using Pd-GaO_3 over amorphous and mesoporous silica supports. The objective of studying gallium oxides is to observe the effects of the different phases of this material (alfa, beta and the combination of alfa-beta) over the catalyst yield for CO_2 hydrogenation.

Keywords: CO_2 Hydrogenation, Pd-GaO_3/SiO_2, Cu-Zn/SiO_2, GaO_3

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral ( ) Poster (X)

Rheology of Rod-like Nanoparticles in Liquid Crystal Polymer Solutions

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ABSTRACT: Liquid crystalline polymers (LCPs) are interesting fluids due to their inherent orientational order and self-organizing properties. Orientation enhances and allows for the control of the mechanical, electrical and thermal properties. Yet, physical properties may be affected by inclusion of particles due to disturbances in the orientation and degree of anisotropy. However, anisotropic particles, such as rodlike nanoparticles, should not significantly affect the phase transition neither the structure of the liquid crystal, due to their geometric similarity with the polymer molecules. In this work, the steady-state viscosity and viscoelastic properties of loaded LCP solutions was determined. The studied systems consist of isocyanate-functionalized multiwalled carbon nanotubes (i-MWCNTs) in poly(*n*-hexyl isocyanate) (PHIC)/*p*-xylene, and either carboxylated multiwalled carbon nanotubes (c-MWCNTs) or halloysite nanoclays (HNCs) in hydroxypropyl cellulose (HPC)/acetic acid aqueous solution. The viscoelastic moduli of the PHIC solution was not significantly affected when up to 5 wt% of i-MWCNTs were dispersed using an ultrasonic bath. The steady-state viscosity increased upon addition of 0.5 wt% i-MWCNTs, irrespectively of dispersion method. For HPC solutions, irrespectively of the dispersion quality, the viscosity and viscoelastic properties of the neat matrix are not to be affected by particle loadings of up to 10 wt% for HNCs and 0.5 wt% for c-MWCNTs. A possible interaction between the nanoparticles and the polymer molecules may be improving the dispersion of the nanoparticles. It have been demonstrated that the length of the rod-like nanoparticles is not a critical parameter in the rheological behavior of a LCP. Results suggest that well-dispersed rod-like nanoparticles do not affect the phase transitions (as verified by microscopy) neither the anisotropic structure of semi-rigid LC polymers.

Keywords: liquid crystalline polymers, rod-nanoparticles, rheology

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral ( ) Poster (✓)

Analysis of the effect of the addition of titanium dioxide to sulfonated poly(styrene-ethylene/butylene-styrene) (SEBS) membranes

Ariangelís Ortiz Negrón, and David Suleiman Rosado
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ABSTRACT: Sulfonated SEBS was functionalized with titanium dioxide (TiO_2) nanoparticles as a possible way to enhance its performance as proton exchange membrane. Different sulfonation levels and TiO_2 quantities were studied. The resulting functionalized polymers were solvent casted and the effects of these functionalizations on the properties of these materials, were evaluated with several materials characterization techniques. In order to quantify and confirm the presence and coordination of the sulfonic groups and the TiO_2 particles, elemental analysis and Fourier transform infrared spectroscopy measurements were performed. The thermal stability of the resulting membranes was determined by thermogravimetric analysis. The results show an increase in thermal stability upon sulfonation. However, the addition of titania nanoparticles had little effect on the degradation temperature of the membranes. In addition, water and methanol swelling of the membranes were analyzed as a function of time in order to determine their absorption limits. Finally, transport properties of the membranes were studied by liquid phase methanol permeability and spectroscopic impedance experiments leading to proton conductivity results. SEBS performance in methanol permeability was similar to the state-of-art Nafion®, while proton conductivities were significantly lower than Nafion®. Additional functionalization of the TiO_2 nanoparticles is currently pursued to create additional proton conducting sites, while maintaining the limited free-volume that inhibits the methanol permeability.

Keywords: poly(styrene-ethylene/butylene-styrene), titanium dioxide, characterization, transport properties

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral (X) Poster ( )

Synthesis of Mesoporous Carbon Catalytic Materials with Improved Thermo Solvent Stability for Dehydration Reactions of Biomass-Derived Feedstocks

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University of Puerto Rico – Mayagüez Campus; Mayagüez, PR

Fossil fuels provide approximately three quarters of today's fuel energy, but current fossil fuel world reserves will not meet future energy demands. Also, the burning of these energy sources is one of the main causes of the increase of CO_2 concentration in the atmosphere that has been associated with Climate Change. Consequently a transition from nonrenewable (fossil fuels) energy sources to renewable energy sources is desirable. Biomass is the main renewable energy source that can substitute fossil fuels, but to achieve this some technical challenges must be solved. One technical challenge is the design of catalysts with good thermo solvent stability. This is especially true for aqueous liquid phase processing, as for example, dehydration reactions of biomass-derived feedstocks that are catalyzed by acids and bases. A possible solution, specifically for dehydration reactions of biomass-derived feedstocks, is the synthesis of carbon materials with high surface areas and acidic functionalities. So far, three different types of Mesoporous Carbon Materials have been synthetized by our group, which area CMK-3, CMK-5, and FDU-15. A phenyl sulfonic acid group has been attached to the surface of CMK-3. Characterization of the materials is being performed using Scanning Electron Microscope (SEM), Nitrogen Adsorption - Desorption Isotherms, and X-Ray Diffraction (XRD). Results to date indicate that the synthesized carbon materials have the desired ordered range of mesopores and textural properties. After functionalization CMK-3 lost its long range ordered mesopore structure. FDU-15 has also been synthesized but the synthesis procedure can still be improved.

Keywords: mesoporous carbon material, dehydration reactions, catalyst stability, acid catalysis

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral ( ) Poster (x)

Development of Iron Oxide Nanoparticles with Enhanced Energy Dissipation for Application in Magnetic Fluid Hyperthermia

Meghan Clardy[1], Dr. Jeremiah Hubbard[1] Dr. Carlos Rinaldi[2]
[1]Department of Chemical Engineering, University of Puerto Rico-Mayagüez
[2]J. Crayton Pruitt Family Department of Biomedical Engineering, Department of Chemical Engineering, University of Florida, Gainesville

ABSTRACT: Magnetic Fluid Hyperthermia has been proven to be an effective method for cancer cell eradication. This technique is based upon cellular uptake of magnetic nanoparticles followed by exposure to an AC field which, through irreversible magnetization dynamics, causes the particles to dissipate energy heating the cell to a temperature high enough to result in programmed cell death. In order to optimize this technique for future medical use, it is vital that the particles respond to the magnetic field in a manner that releases the most energy. Optimal heat dissipation in a fixed medium is achieved by maximizing the Neél relaxation losses, resulting in increased energy dissipated due to internal dipole rotation. Iron Oxide Nanoparticles (IONPs) have the potential to improve the MFH process greatly because magnetite would be a desirable alternative to toxic Cobalt, and their lower magnetic anisotropy energy results in the dominance of Neél relaxation. Neél relaxation times are dependent upon the magnetic diameter of the particles, with an ideal magnetic diameter for energy dissipation between 16-19nm. IONPs of this size have been synthesized using a high boiling point solvent in a monitored thermal decomposition reaction. Successful syntheses have demonstrated that optimal diameter IONPs dissipate tenfold the energy in comparable AC fields than monodisperse IONPs with magnetic diameters less than 10nm. Designing and functionalizing these targeted particles that can dissipate elevated amounts of energy would improve this technique by making the mechanism more efficient in heating with less particles needed at the targeted cancer tissue.

Keywords: Iron Oxide Nanoparticles, Magnetic Fluid Hyperthermia, Particle Energy Dissipation, SAR

ABSTRACT

UPRM Chemical Engineering
Graduate Research Fall Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral (X) Poster ()

The effect of particles with asymmetric friction coefficient to the flowability of granular materials

Efraín Y. Aymat and Ubaldo M. Córdova-Figueroa
Department of Chemical Engineering, University of Puerto Rico-Mayagüez

ABSTRACT: A set of discrete particles large enough that inertia and gravity becomes important is also known as granular media. The peculiarity of studying these materials is the multiple observed behaviors depending on their volume fraction. At the solid state (high volume fractions), many studies have focused in understanding the flow characteristics and properties of particles by changing the surface cohesivity through a lubricant. However, it has been shown experimentally that particle lubrication leads to low uniformity, poor distribution and undesired amount of lubricant on the carrier particles, which induce unexpected flowability properties. This uneven distribution of lubricant has not been taken into account in current models and it is the subject of our study. To understand this material at a particle level, an event driven simulation based on hard-sphere interactions is constructed. The effect of asymmetric friction coefficient in particles on the tensor stress, velocity profile, particle density, and other relevant physical properties will be investigated. Further knowledge and utilization of asymmetrically functionalized particles could contribute greatly to the performance of more realistic simulations of manufacturing processes and the creation of smart granular materials.

Keywords: cohesivity, hard sphere, inelastic collapse, granular media, Janus Particles

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral ( ) Poster (X)

Flavoring Effect on the Thermal Gelation of HPMC Physical Gels

Carlos Pinzón – Aldo Acevedo
Department of Chemical Engineering, University of Puerto Rico-Mayagüez

ABSTRACT: Understanding of the gelation process of pharmaceutically relevant physical gels is necessary to optimize formulations and processes, as well as to discern gelation mechanisms. In this study we evaluate the effect of twelve flavoring agents on the physical gelation temperature of 1wt% hydroxypropyl methylcellulose (HPMC) solutions in a water-ethanol mixture. The flavoring agents were organized by its principal functional group, i.e. alcohols, esters, monoterpenes, and aldehydes, and concentrations of up to 0.1 wt% were characterized. Rheological dynamic oscillatory measurements with temperature ramps from 20 to 80 °C were used to determine the gelation temperature, T_{gel}. All measurements were made in triplicate and a variance analysis (ANOVA) for each functional group was performed, to determine the effect of concentration and type of flavoring. Results show that both factors, type of molecule and concentration, have a significant effect on the gelation temperature of the samples. Special cases observed were monoterpenes and ester groups, where no discernible pattern was identified. The Flory-Huggins solubility parameters were used to correlate the effect of different flavors in the gelation temperature of the system. A relationship between the solubility of the flavoring with the solvent and polymer can be correlated to the changes in T_{gel} of the HPMC solutions.

Keywords: Tgel, HPMC, drug delivery, gelation.

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral (X) Poster ( )

Rheology of Hard-sphere and Square-well Suspensions by Brownian Dynamics Simulation

Ronal De La Cruz-Araujo and Ubaldo M. Córdova-Figueroa
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ABSTRACT: Recent experimental and theoretical studies on the suspension of patchy or Janus colloidal particles (JCPs) have examined collective structures, phase diagrams, and self-assembly at different times scales and particle concentrations. However, only a few efforts have focused on understanding their potential rheological advantages in comparison to their isotropic counterparts. Our general plan is to evaluate the rheological behavior of a suspension of JCPs subject to a simple shear flow. Therefore, we propose a model system consisting of a monodisperse colloidal suspension, composed of JCPs immersed in a Newtonian fluid interacting with other JCPs via a combination of square-well (SW) and hard-sphere (HS) surface potentials that depend on their relative orientation and distance. In this work, we present rheological studies for two systems equivalent to JCPs suspension, but with isotropic particles, interacting between them with only HS or with only SW surface potentials, using Brownian dynamics simulation. These studies for simple systems are carried out in order to validate our simulation method and to compare the results with our future results for a complex system of JCPs and to observe their principal differences. Rheological properties, such as osmotic pressure, microstructure, effective suspension viscosity, and normal stress differences, are obtained and validated for HS and SW suspensions at equilibrium and away from it, respectively, as a function of the Péclet number *Pe* and particle volume fraction. As expected, the effective viscosity shows shear thinning as *Pe* is increased and a growing osmotic pressure as a function of volume fraction. The SW suspension, in general, does not reach equilibrium due to formation and break-up of clusters over time. The clusters are characterized at each time interval by measuring the number of clusters, the number of particles in each cluster, the radius of gyration, and the cluster effective size. These cluster properties are used to explain the time-dependent rheological properties of the SW suspension.

Keywords: Square-well suspension, Janus particles, rheology, microstructure, colloidal suspension

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral ( ) Poster (x)

Synthesis and Characterization of a Polysiloxane Based Liquid Crystalline Elastomer

Stephany Herrera Posada, Aldo Acevedo, Barbara Calcagno
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ABSTRACT: Liquid crystalline elastomers (LCE´s) are liquid crystal polymers which combine mechanical orientability of rubbers with the ordered structure and mobility of LC phases. They have special optical, mechanical and piezoelectric properties and are able to change these properties in response to external stimuli, offering potential applications as mechanical actuators, in optics and sensing. In this work, we propose to improve the sensitivity of these elastomers to external stimuli by triggering mechanical and optical responses through external magnetic fields or visceversa. In order to do this, we are developing comoposites based on the introduction of chemically functionalized magnetic particles.

Polysiloxanes are ideal candidates due to their biocompatibility and known chemical synthesis and modification and, the liquid crystalline elastomer proposed consist of a polysiloxane backbone (poly(methylhydrosiloxane)); a mesogenic pendant group (4-methoxyphenyl-4´-allyloxybenzoate) and a bifunctional crosslinker (1,4-bis(undecyl-10-enyloxy)benzene). Preliminary results for the synthesis and characterization by differential scanning calorimetry, infrared spectroscopy, nuclear magnetic resonance spectroscopy and polarized optical microscopy of the precursors and the liquid crystalline elastomer will be presented.

Keywords: liquid crystal elastomer, magnetic composites, polysiloxane

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral ( ) Poster (x)

Adsorptive Removal of Carbamazepine and Salicylic Acid from Water Using a Zeolite Modified with Extraframework Transition Metal Cations and a Surfactant

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[b]*Department of Chemistry, University of Puerto Rico,Mayagüez Campu.*

ABSTRACT: Pharmaceutical and Personal Care Products (PPCPs) are considered emerging contaminants that present great challenges for their remediation from water. However, adsorption processes based on microporous materials could offer an efficient solution if tailored properly. In this study, the adsorptive removal of two emerging contaminants (salicylic acid and carbamazepine) from an aqueous solution was accomplished using a Faujasite-type synthetic zeolite modified with transition metals and a surfactant moiety. Co^{2+}, Cu^{2+} or Ni^{2+} were employed to induce complexation-like adsorbate-adsorbent interactions at ambient conditions in an attempt to provide an efficient removal driving force in the low ppm range. The use of a surfactant is of utmost necessity given the highly hydrophilic nature of the zeolite. However, the adsorption equilibrium data clearly showed that the best capacities are obtained when a transition metal/surfactant combination is employed.

Keywords: Adsorption, transition metals, zeolite, PPCPs

ABSTRACT

UPRM Chemical Engineering
Graduate Research Spring Symposium

University of Puerto Rico-Mayagüez
Friday, May 3, 2013

Check one: Oral (x) Poster ( )

Synthesis of a novel polyether block copolymers for fuel cells and specialty separations applications

Maritza Pérez_Pérez and David Suleiman_Rosado
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ABSTRACT: This investigation describes the synthesis and characterization of novel polyether polymers for fuel cells and specialty separations. The polyethers with novel functional groups and entropically hindering moieties were synthesized via cationic polymerization. These polymers have been characterized using: Fourier Transform Infrared Spectroscopy (FT-IR), Differential Scanning Calorimetry (DSC), Thermo-gravimetric Analysis (TGA) and Gel Permeation Chromatography (GPC). The main block copolymer studied was Poly(Isobutylene-Styrene-Ethylmethylether-Styrene) (ISES). This novel copolymer is considered as an alternative to solve two of the main challenges society faces in the 21st century: Energy and the Environment. ISES could address both challenges by using less energy intensive membrane separation processes and allowing selective permeation in fuel cell devices, creating more efficient environmentally benign alternative energy sources.

Keywords: Cationic polymerization, fuel cell, polyethers, environment and energy