Twelfth Annual Chemical Engineering Graduate Symposium

February 22, 2011
Particle Engineering Research Center Particle Science and Technology
– Room 202
http://grace.che.ufl.edu
Eleventh Annual Chemical Engineering Graduate Symposium

8:45 – 8:50  Welcome and opening remarks  
              Rafe Biswas, (Academic Chair) and Poom Buncha (President).

Session I – Material Sciences

8:50 – 9:15  Jose Angel Hinojosa  
             Dr. Jason Weaver  
             Chemistry and Surface Characterization of PdO(101)

9:20 – 9:45  Hongta Yang  
             Dr. Peng Jiang  
             Self-Cleaning Macroporous Films by Doctor Blade Coating

9:50 – 10:15  Rob Colymer  
              Dr. Helena Hagelin-Weaver  
              The Use of Nanoparticle Oxides as Supports for Cobalt-Based  
              Fischer-Tropsch Catalysts

10:20 – 10:45  Wei-han Huang  
               Dr. Peng Jiang  
               Bioinspired strong graphene oxide composite

10:45 – 11:00  Break

Session II - Study of Fluids

11:00 – 11:25  Casey Lamarche  
               Dr. Jennifer Sinclair Curtis  
               Subsonic cratering of a particle bed

11:30 – 11:55  Cheng-Chun Peng  
               Dr. Anuj Chauhan  
               Extended Ophthalmic Drug Delivery by Silicone Contact Lens  
               Containing Vitamin E

12:00 – 12:25  Akhil Rao  
               Dr. Jennifer Sinclair Curtis  
               Numerical Simulation and Validation of a Dilute Turbulent Gas-  
               Particle Flow Model with Turbulence Modulation

12:30 – 1:30  Lunch

Session III – Biological Sciences
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The oxidation of transition metal surfaces involves the development of a variety of oxygen states, which can have distinct properties. In particular, different surface oxygen states can have unique reactive properties that could dramatically alter the catalytic behavior of a transition metal surface. Preparing well ordered oxygen states can provide the opportunity to gain further insights into these properties. I will discuss the structural effects observed through scanning tunneling microscopy (STM) of a decomposing bulk like PdO(101) thin film grown on a Pd(111) surface under ultrahigh vacuum (UHV) conditions. We observe that PdO(101) grows in a patch like network that is well distributed across the surface. Upon annealing the PdO(101) surface, the patch like network is replaced by large well ordered islands. We also observe several types of oxygen domains during decomposition of the PdO(101) thin film, which gives insight into the atomic-level mechanisms governing oxide reduction. I will also discuss the molecular adsorption and dissociation of n-butane on a PdO(101) thin film. By using temperature-programmed reaction spectroscopy (TPRS) experiments we observe that n-butane adsorsbs on PdO(101) in a molecular state that is more strongly-bound than n-butane physisorbed on Pd(111). We show that this molecularly adsorbed state of n-butane corresponds to a s-complex that forms on the rows of coordinatively unsaturated (cus) Pd atoms of the oxide surface. I will also present evidence that that adsorbed s-complexes play a general role as precursors in alkane activation on transition metal oxide surfaces.

About the Speaker:

Jose received his Bachelors of Science in chemical engineering with a minor in Chemistry from the University of Houston in May 2005. Jose joined the Department of Chemical Engineering at the University of Florida in August 2005, and then joined the Weaver research group in December 2005.

Tension generation in endothelial cells is necessary for normal cell function. Tensile force within non-muscle tissue cells is generated in actomyosin stress fibers, which are composed of contractile units called sarcomeres. The mechanics and dynamics of sarcomeres are not well understood due to the lack of experimental measurements in the living endothelial cells. Using femtosecond laser ablation, we severed living stress fibers and measured sarcomere contraction under zero tension. From these novel experiments and modeling we proposed a new mechanical model for tension generation where the force in the stress fiber is balanced entirely by actomyosin forces in each sarcomere. Through live cell imaging we observed that the number of sarcomeres and sarcomere lengths dynamically change in the cell. We show that sarcomere lengths continually fluctuate, with a fluctuation relaxation time of about 20 minutes. New sarcomeres are formed at focal adhesions and are convected into the fiber at a speed that is independent of focal adhesion size, suggesting that the speed is independent of tension. Furthermore sarcomeres were observed to disappear at specific points or “sinks” along the stress fibers. These results show that stress fibers are highly dynamic structures despite their relatively static morphology, with nascent sarcomeres forming and being incorporated into the fiber at a nearly uniform, tension-independent velocity throughout the cell. The fluctuating length of individual sarcomeres under constant tension is consistent with our mechanical model whereby sarcomere contraction/expansion speed, rather than sarcomere length, is modulated by tension.

About the Speaker:

Robert received his Bachelor of Science in chemical engineering and biomedical engineering from Carnegie Mellon University in May 2006. He then joined the Department of Chemical Engineering at the University of Florida in August 2006 and began working under Professors Tanmay Lele and Richard Dickinson in January 2007.
Recent studies of neuron development and cell migration suggest that nucleus translocation is a highly coordinated event associated to several cell activities. For example, the nucleus of a cell has been observed to possess a rearward translocation when the cell starts migrating at the edge of a wound. Based on these phenomena, we have developed an image analysis method to correlate the cell and nucleus centroid movements by analyzing microscopic images of single cells. Image analysis reveals significantly different correlation patterns between the centroid of the nucleus and the centroid of cell upon manipulation of the activation levels of the Rho GTPase family proteins, which are the critical signaling proteins to regulate cell motility and include RhoA, Rac1, and cdc42. Based on our study, microscopic image analysis of one-hour single cell video may extract the cell migration status and distinguish the different signaling pathways that control cell migration.

About the Speaker:

PhD Candidate - University of Florida, Gainesville, FL
Chemical Engineering, Aug. 2007 – Aug. 2011 (Expected)

M.S. - National Taiwan University, Taipei, Taiwan

B.S. - National Taiwan University, Taipei, Taiwan

Self-Cleaning Macroporous Films by Doctor Blade Coating

Here we report a scalable bottom-up technology for creating three-dimensionally highly ordered macroporous polymer films with excellent water-repelling and optical diffractive properties. A simple doctor blade coating process is first utilized to create silica colloidal crystal-polymer nanocomposites. The close-packed silica spheres are selectively removed to fabricate flexible macroporous polymer films with crystalline arrays of voids which are interconnected through small nanopores. The size of the voids can be easily controlled by tuning the duration of an oxygen reactive-ion etching process prior to the removal of the templating silica spheres. After surface functionalization with fluorosilane, superhydrophobic surface with large apparent water contact angle and small sliding angle can be obtained. The waterrepelling property can be quantitatively explained by adapting the Cassie’s dewetting model. We further demonstrate that self-cleaning functionality can be achieved on superhydrophobic macroporous coatings by preventing bacterial contamination.

About the Speaker:

Hongta Yang received a bachelor’s degree in Chemical Engineering from National Taiwan University in 2001, and a master degree in Chemical Engineering from Georgia Institute of Technology in 2008. He began his graduate studies at the University of Florida in August 2008 and joined Professor Peng Jiang’s nanostructured material research group to pursue a doctorate degree.
The Use of Nanoparticle Oxides as Supports for Cobalt-Based Fischer-Tropsch Catalysts

Robert Colymer
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Dr. Helena Hagelin-Weaver

In our investigation a fixed bed reactor system was used to test our catalysts. Several catalysts were prepared using the incipient wetness impregnation method of cobalt precursors onto nanoparticle and porous silica, titania, and alumina supports. These catalysts were subjected to Fischer-Tropsch reaction conditions, in which CO and H2 are converted to hydrocarbons at a pressure of 20 bars and temperatures in the range of 210 to 250°C, to determine the differences in CO conversion and selectivity to liquid hydrocarbons between catalysts supported on nanoparticle and porous oxides. The use of promoters, both oxide and noble metal promoters, were also investigated to determine if the choice of optimal promoter is dependent on whether the nanoparticle oxides or porous supports are used. The catalysts were characterized using a number of analytical techniques, such as BET to determine the overall catalyst surface area, CO chemisorption to determine Co metal surface area, temperature programmed reduction (TPR) to determine the reduction properties of the catalyst, X-ray diffraction (XRD) to determine the crystal structure and size of the catalyst components. Initial results reveal that the porous silica (Alfa Aesar) gives a higher conversion and a higher selectivity towards liquid hydrocarbons than the nanoparticle silica (NanoScale). In general, the titania-supported catalysts required higher temperatures in our experiments to show CO conversions comparable to the silica supported catalysts. Initial results indicate that nanoparticle titania (NanoActive) performs better than porous titania (Alfa Aesar). Work in progress involves using different promoters with the nanoparticle supports to increase the activity and selectivity to the diesel fraction.

About the Speaker:

I am from the Philadelphia, Pennsylvania Area. I have a Bachelor’s Degree in Chemical Engineering from The Pennsylvania State University, a Master’s Degree in Chemical Engineering from Villanova University. This is the end of my fourth year here.

A Model for Fluctuating Torque on the Nucleus

Jun Wu
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Dr. Tanmay Lele

In living cells, a fluctuating torque is exerted on the nuclear surface but the origin of the torque is unclear. In this study, we found that the nuclear rotation angle is directionally persistent on a time scale of tens of minutes, but rotationally diffusive on longer time scales. Rotation required the activity of the microtubule motor dynein. We formulated a model based on microtubules undergoing dynamic instability, with tensional forces between a stationary centrosome and the nuclear surface mediated by dynein. Model simulations suggest that the persistence in rotation angle is due to the transient asymmetric configuration of microtubules exerting a net torque in one direction until the configuration is randomized by dynamic instability. The model predicts that the rotational magnitude must depend on the distance between the nucleus and the centrosome. To test this prediction, rotation was quantified in patterned cells in which the cell’s centrosome was close to the projected nuclear centroid. Consistent with the prediction, the angular displacement was found to decrease in these cells relative to unpatterned cells. This work provides the first mechanistic explanation for how nuclear dynein interactions with discrete microtubules emanating from a stationary centrosome cause rotational torque on the nucleus.

About the Speaker:

I received my BS degree in Chemical Technology and MS degree in Chemical Engineering from Tianjin University, China. I joined Department of Chemical Engineering at the University of Florida in August 2007, and then joined Dr. Tanmay Lele’s group in October 2007. My research is focusing on understanding nuclear movement in mammalian cells and mechanics of cytoskeleton.
Numerical Simulation and Validation of a Dilute Turbulent Gas-Particle Flow Model with Turbulence Modulation

Akhil Rao
akhil-rao@hotmail.com
Dr. Jennifer Sinclair Curtis

This work presents a numerical study of a dilute turbulent gas-particle flow with inelastic collisions and turbulence modulation in an Eulerian framework. A new interpretation is provided for the interaction/coupling terms, based on a fluctuating energy transfer mechanism. This provides for a new robust closure model for the interaction terms with the ability to predict the turbulence dampening as well as the turbulence enhancement phenomena. Further, the model developed herein is investigated along with a variety of other published closure models used for the interaction/coupling terms, particle drag and solid stress. The models are evaluated with several sets of benchmark experiments for fully-developed, turbulent gas-solid flow in a vertical pipe.

Bioinspired strong graphene oxide composite

Wei-han Huang
weha.huang@gmail.com
Dr. Peng Jiang

Nature shows great design that combine plateletlike ceramic building block with polymer matrices to become the hybrid material of high strength and flaw tolerance. Those particular structures of nature materials and their concepts of their mechanical behaviors have been extensively studied. Now inspired by nature, we assemble graphene oxide sheet, one of the most strong-stiff material on earth, as building block and combine with PVA polymer via infiltration to synthesize nanocomposite with unique strength and ductile.

About the Speaker:

Wei-han Huang (Erik) is from Taiwan, got his Bachelor degree in Chemical Engineering in National Taiwan University in 2003. He studied in UF since 2006 and joined Dr. Peng Jiang’s group in 2007. His researches focus on nanoparticle self-assemble and reinforced nanocomposite.

About the Speaker:

Birthdate: 1/12/1986
Birthplace: Mumbai, India
Undergraduate School: Institute of Chemical Technology, Mumbai, India
PhD. degree (Work In Progress): University of Florida
Subsonic cratering of a particle bed

Casey Lamarche
Casey.lamarche@gmail.com

Dr. Jennifer Sinclair Curtis

Future space exploration necessitates improved gas-solid and solid-solid interaction models. Impinging rocket plumes from spacecraft interact with the lunar regolith surface and release a high velocity particle-spray that is potentially hazardous to surrounding surface structures and surface architecture. Experiments performed at NASA-KSC provide data on the cratering of a particle bed by a turbulent subsonic jet of gas. In order to model this system, an Eulerian treatment is employed using locally averaged equations of motion along with closure relations describing the solids-phase stress derived using concepts based on dense-phase gas kinetic theory. The solids phase frictional stresses, which occur at high solids volume fractions and result from sustained particle-particle contacts, are based on critical state theory. Standard commercial codes employ these frictional stress models, but poorly predict the cratering dynamics found experimentally and predict a particle bed that is too liquid-like. However, a continuum frictional stress model in which the normal frictional pressure and frictional viscosity is increased significantly improves the predictions for the cratering behavior. In addition, the effect of the changes in the jet velocity, density, diameter, and height are explored and compared with experimental data for crater width and depth.

About the Speaker:
Not Provided

Extended Ophthalmic Drug Delivery by Silicone Contact Lens Containing Vitamin E

Cheng-Chun Peng
cpeng@gmail.com

Dr. Anuj Chauhan

Ophthalmic drug delivery via eye drops is inefficient as only 1-5% of the applied drug enters the cornea and the rest is absorbed into the bloodstream, which could cause side effects. Furthermore, application of ophthalmic drugs as drops results in a rapid variation in drug delivery rates to the cornea that limits the efficacy of therapeutic systems and limit compliance. The purpose of our research is to develop soft contact lenses containing Vitamin E for long term and controlled drug delivery to eliminate these problems.

The hydrophobic Vitamin E is loaded into commercial silicone contact lens by being dissolved in ethanol that swells the lens and subsequently forming aggregates inside the lens after solvent evaporation. In vitro results showed that the increase in release duration is quadratic for hydrophilic drugs (Timolol, fluconazole and dexamethasone phosphate) in Vitamin E loading. For hydrophobic dexamethasone, the effect of the Vitamin E inclusion is smaller but still significant for release. The ocular drugs delivery by contact lens can be viewed as a one-dimensional transport by a flat thin film, and subsequent mathematical models were established based on the increase of diffusion path length for hydrophilic drugs and the low diffusivity in the Vitamin E aggregates for hydrophobic drugs. Furthermore, incorporation of Vitamin E does not disqualify these silicone hydrogels as extended-wear contact lens with appropriate oxygen and ion permeability. In addition, Vitamin E loading has a beneficial effect of blocking UV radiation which will reduce the corneal damage due to UV light.

About the Speaker:
PhD Candidate
University of Florida, Gainesville, FL
Chemical Engineering
Aug. 2007 – Aug 2011 (Expected)