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Book of Abstracts

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AIChE Midwest Regional Conference

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AIChE Midwest Regional Conference
Presentation Abstracts
Tuesday, February 28, 2017

Biofuels
Tuesday, February 28, 2017 (Cardinal Room, **TueA1**)
Chair: *Victor Sussman* (Dow Chemical)
Co-Chair: *Mustafa Cagdas Ozturk* (Illinois Tech)

9:45 AM **Comprehensive Generation of Libraries of Lignin Structures as an Exploration of Lignin Space** (TueA1a)
Lauren Dellon, Linda Broadbelt (Northwestern University), *Wenjun Li, Ross Mabon* (ExxonMobil)

The structure of lignin has yet to be entirely understood owing to its polydispersity, complexity, and hyperbranched topology. In previous work, the Broadbelt group has developed an algorithm capable of generating libraries of structural representations of wheatstraw lignin whose average properties – monomer distribution, bond distribution, molecular weight distribution, and branching coefficient – statistically agree with the experimental values. In this work, we have extended this stochastic method to accommodate more complexity, in addition to any type of biomass – softwood, hardwood, or herbaceous. The individual lignin molecules were constructed by random walks along decision trees, where the structure of the trees and the values of the edge weights were informed by unique structural and mechanistic details. With the additional complexity, two methods were investigated and ultimately utilized to reduce the degrees of freedom of the optimization of the edge weights. The first method was pruning the decision trees so as to have fewer parameters, and the second method was biasing the edge weights to within a certain range of their experimental values so as to decrease the size of the parameter space. Utilizing these two methods, we were able to obtain edge weights that produced libraries for miscanthus (herbaceous), spruce (softwood), and birch (hardwood). Notably, wheatstraw and beech proved problematic, revealing that drawing experimental values from disparate sources may lead to a combination of properties that cannot be physically realized. Building on these results, we put forth the concept of feasible “lignin space”, i.e., ranges of experimental characteristics quantified by the four main properties above that can be realized simultaneously. Thus, the advantages of the approach are twofold: generation of lignin libraries for any biomass source to be used in kinetic modeling studies, and guidance for experimentalists as they seek to design and characterize lignin.

10:05 AM **Hydrothermal Liquefaction (HTL) of High-ash Algal Biomass: the Effect of Ash Contents in HTL Reactions** (TueA1b)
Wan-Ting Chen (University of Illinois at Urbana-Champaign)

Previous studies demonstrate that the high ash contents in the hydrothermal liquefaction (HTL) processes appeared to retard the formation of biocrude oil. HTL tests of high-ash algal biomass were conducted in this study to understand the role of ash contents under the HTL processes. Mixed-culture algal biomass from wastewater systems (AW) were screened into three sizes (<106 µm, 106-180 µm and >180 µm) and their ash contents were measured. AW biomass with different ash contents was converted into biocrude oil via HTL at 300 ˚C for a 60 minute reaction time, which is the previously determined optimum condition for producing biocrude oil from AW. Compared to AW biomass before screen pretreatments, the ash contents of AW of 106-180 µm and <106 µm were respectively decreased from 53.3 % to 38.5% and 41.8 %, while the biocrude oil yields remained almost constant. When the ash contents were reduced from 53.3 % to 38.5 % in the AW biomass, the HHV of biocrude oil was increased from 27.5 MJ/kg to 32.3 MJ/kg and the fraction of light oil (boiling point of 100-300 ˚C) was increased from 31% to 49%. On the other hand, GC-MS analyses of algal biocrude oil and aqueous products show that the ash contents could promote denitrogenation, catalyze the formation of hydrocarbons, as well as mitigate the recalcitrant compounds in aqueous products under the HTL processes. Based on the above results, it is hypothesized that algal biomass with certain amounts of ash contents can be converted into reasonable quality and quantity of biocrude oil and more degradable HTL aqueous products for microorganism growth. In order to quantify the limit of the ash contents under the HTL processes, further HTL conversions with model algal feedstock and representative ash contents were conducted in this study. Elemental and thermogravimetric analyses of the resulting biocrude oil both demonstrate that when the ash content in the algal feedstock was below 40%, the HHV and boiling point distribution of the algal biocrude oil could be hardly affected. This fact substantiates the feasibility of using high-ash algal biomass as HTL feedstock and diminishes the necessity of multi-step pretreatments and modifications of high-ash biomass for biofuel application.

10:25 AM **Organic Waste Management: Modeling and Decision-Making Strategies** (TueA1c)
Apoorva Sampat, Victor Zavala (University of Wisconsin Madison)

We propose a modeling abstraction for multi-product supply chains that we use to analyze dependencies between products and make design decisions regarding technology selection and placement. Our framework uses a compact representation of dependencies using a general yield factor matrix that maps technology performance to input and output products. We show how to use this formulation to create coherent models in a wide range of potential applications. We demonstrate the capabilities using a case study on phosphorus and biogas recovery from organic waste in the State of Wisconsin.

10:45 AM **Using the Best of Biology and Chemistry for Sustainable Solutions** (TueA1d)

Mike Schultz (*PTI Global Solutions*)

While fuels and chemicals continue to be predominately produced by conventional, thermochemical means, bio-based routes are growing in importance. As bio-based process technology and supporting tools become more relevant at scale, a trend is developing in which hybrid systems couple a thermochemical conversion process with a biological conversion process, leveraging the advantages of each. Examples include thermal conversion of biologically derived materials such as biomass and vegetable oils to produce fuels and chemicals directly, thermal conversion of biological materials to prepare a feedstock suitable for a biological process, and thermochemical conversion of biologically produced alcohols and organic acids to produce drop-in fuel and chemical products.

This presentation will review both commercial and emerging examples of such coupled systems, and demonstrate the advantages of each, along with caveats and limitations. Finally, comments on future directions of such systems will be presented.

11:05 AM **Application of a Simultaneous Biogas Production and Upgrading Process for Renewable Methane Production using Municipal Sludge in Laboratory- and Pilot-Scale Digesters** (TueA1e)

Meltem Urgun-Demirtas (Argonne National Laboratory)

Renewable methane production takes an increasing momentum in the light of stringent discharge criteria and high tipping fee for disposal of organic waste streams. Meanwhile, biogas production technology has been playing an important role in achieving the renewable fuel volume targets set by the US EPA [1]. The present abstract aims to develop a sustainable and efficient platform for production of renewable methane and value-added fertilizer at wastewater treatment plants.

We recently reported an integrated waste-to-energy system for anaerobic digestion (AD) of municipal sewage sludge with pyro-biochar and achieved pipeline-quality renewable methane by performing the shake flasks experiments under batch mode [2, 3]. In this work, this novel process was scaled up to two-stage AD systems operated under semi-continuous mode, which was demonstrated in 0.5-L and 14-L digesters respectively. In 0.5-L digesters, the performance of thermophilic AD of sludge amended with two types of pyro-biochar (corn stover biochar (CSBC) and pine biochar (PBC)) was compared to the control without biochar under different operational conditions. CSBC and PBC both improved the performance of AD in terms of substrate utilization, methane production rate and process stability and CSBC showed superior performance. The maximum methane purity in biogas (95%) and methane yield (0.34 L/g VS-added) were achieved with CSBC addition. The response surface methodology (RSM) modeling results showed that biochar loading and organic loading rate were two significant parameters for optimization of the semi-continuous thermophilic AD process. Depending on the dosage and biochar type, the biochar supplementation also substantially increased multiple macro- (N, P, K) and micro-nutrients (Ca, Mg, Fe) in the resultant digestate by up to 2600% to enhance its fertilizer value. Furthermore, the biochar addition, particularly CSBC, promoted the relative abundance of Clostridia and Methanosarcina among the microbial community in the digester, which would facilitate production of the key intermediate acetate and methanogenic activity. The 14-L digester system was used to further evaluate the practical effectiveness of such a thermophilic AD process. Overall, the AD process with CSBC addition outperformed the control by 19% and 35% in terms of methane purity and methane productivity, respectively. The maximum methane purity of 83% and methane productivity of 0.37 L/g VS-added were achieved during steady-state operation with the CSBC loading of 2.1 g biochar/g VS. Collectively, this study proves that biochar addition enhances the AD performance at lab scale (0.5 L) and pilot scale (14 L) and has a great potential to commercially produce renewable methane with high productivity and reduce or minimize the need for biogas cleanup as well produce high fertilizer value digestate from organic waste streams.

References:

1. https://www.epa.gov/renewable-fuel-standard-program/program-overview-renewable-fuel-standard-program
2. Shen et al. (2015) Applied Energy, 158: 300-309
3. Shen et al. (2016) Journal of Cleaner Production, 135:1054-1064

<u>Process Modeling and Optimization</u>

Tuesday, February 28, 2017 (White Oak, **<u>TueA2</u>**)

Chair: *Belma Demirel* (Guidepoint)

Co-Chair: *Jeffrey M. Zalc* (BP)

9:45 AM **Semi-Empirical Modeling of Capacity Fade: A Practical Approach for Battery Pack Manufacturers** (TueA2a)

Bader Jarai, Stephen K. Wilke, Ben Schweitzer, Siddique Khateeb, Said Al-Hallaj (AllCell Technologies)

The growing demand for lithium ion batteries with long lifetime and warranty presents significant challenges for battery pack manufacturers to sufficiently understand cell ageing while keeping testing and validation costs low. To ensure the feasibility and competitiveness of Li-ion batteries in industrial applications, it is imperative for battery manufacturers to utilize the most up-to-date cell technologies and, at the same time, guarantee its fulfillment of lifetime requirements. To keep up with the rapid deployment of new cell types, appropriate modeling can be used to extrapolate limited-duration empirical results. We have implemented a semi-empirical modeling approach for predicting capacity fade under various operating conditions, using physics-based degradation mechanisms that provide a good fit to experimental data. Based on a specific product applications, an experimental matrix was designed to illustrate the effects of temperature, depth-of-discharge (DOD), time, and energy throughput on calendar and cycle ageing. Good agreement between the model and empirical results is demonstrated for two state-of-the-art 18650 cell types. The major improvement of this work over other approaches is that it minimizes the testing necessary to validate the unique capacity fade of each new cell type, allowing pack manufacturers to rapidly and accurately down-select the best candidate cells for specific applications.

10:05 AM **Mathematical Modeling and Simulation of Nucleation and Growth of Crystalline Polymorphs** (TueA2b)

Anish Dighe, Meenesh Singh (University of Illinois at Chicago)

Ability of a compound to exist in more than one solid state is known as polymorphism, which is frequently observed during crystallization of pharmaceutical molecules. Bioavailability of a pharmaceutical compound depends on the physical properties of the crystalline form such as dissolution rate and stability. Spontaneous structural changes in this solid state can lead to decrease in the bioavailability and hence efficacy of a drug. It is important to understand the structural transformation in the crystalline materials during the crystallization process to prevent such undesired effects. Crystallization is a process of self-assembly of solute molecules which leads to formation of crystal nuclei followed by their growth in a super-saturated solution. The current approaches to predict the structure of crystal nuclei are lattice energy minimization, molecular dynamics, and kinetic Monte Carlo methods. These approaches have been used to model self-assembly, nucleation and crystal growth processes. There is a need for a multi-scale modeling and simulation to understand and control the crystal nucleation and growth processes beyond the length and time scales spanned by foregoing approaches. In this talk, I will review the existing techniques used for crystal structure prediction, and various models that used for self-assembly, nucleation and crystal growth. I will also present a multi-scale scheme to model of crystallization processes.

10:25 AM **Modelling and Analysis of Solvent Drying in Li-ion Battery Electrodes** (TueA2c)

Naresh Susarla, Shabbir Ahmed, Dennis Dees (Argonne National Laboratory)

In this work, we study and analyze the design aspects and energy requirements of solvent removal and drying in the electrode processing step of Lithium-ion battery production. The heat for the drying is derived from a combination of infra-red (IR) radiators and hot air injectors. We develop a mathematical model of the physical phenomena to understand the various factors affecting the drying rate. The solvent removal involves simultaneous heat and mass transfer with phase change. Our model considers capillary flow and gravity effects for liquid transport and diffusion for vapor phase transport. The model also accounts for the shrinkage of coating thickness with the removal of the solvent. The system of non-linear partial differential equations is then solved numerically using a finite element method to predict the concentration and temperature profiles within the drying cathode layer. We finally study the effects of various factors such as drying temperatures and air conditions on the process performance.

10:45 AM **Molecular Modeling of Liquid-Liquid Phase Equilibria in Ternary Systems** (TueA2d)

Xiaoyu Wang, Sohail Murad (Illinois Tech)

We report simulations results for liquid-liquid equilibria for a ternary mixture of cyclohexane, water and methanol. We have used the "Transferable Potentials for Phase Equilibria (TraPPE)" force field to model the components in this phase equilibrium simulation. The results are compared with recently measured experimental data reported by NIST. We model this system using a novel technique developed by us earlier to measure solubility of gases in liquids. We use an imaginary membrane which is permeable to some components and impermeable to other components. The TraPPE force field will be adjusted if necessary to enable better agreement with experiments.

11:05 AM **A Graph-Based Framework for Hierarchical Modeling and Optimization of Complex Systems** (TueA2e)

Jordan Jalving, Victor Zavala (University of Wisconsin-Madison)

This talk presents a graph-based modeling framework that facilitates the construction and analysis of coupled, structured optimization models. To do this, it leverages a hierarchical graph abstraction wherein nodes and edges can be associated with mathematical models and connectivity constraints (physical or logical). Given a graph structure with models and connections, it can produce either a pure (flattened) optimization model to be solved using any off-the-shelf optimization solver, or it can communicate structures to parallel solvers. Additionally, by using a graph abstraction, a model can be created in collaboration where different modelers develop different components. The hierarchical graph abstraction also induces hierarchical data structures, which makes input and output data easier to parse and analyze.

Fluid Dynamics and Transport Phenomena I

Tuesday, February 28, 2017 (Illinois C, **TueA3**)

Chair: *Lewis E. Wedgewood* (University of Illinois at Chicago)

Co-Chair: *Matthew Liberatore* (University of Toledo)

9:45 AM **Evaluation of an Oscillatory Baffled Reactor for Crystallization Systems** (TueA3a)

Claire Y. Liu, Zoltan Nagy (Purdue University), *Alastair Barton, Paul Firth* (Alconbury Weston Ltd)

In the current pharmaceutical industry, crystallization has become the key step to tune drug properties like solubility and bio-availability. Efficient transport of mass and energy and good fluid mixing are essential in crystallization processes to ensure uniform product quality. Traditionally, crystallization is achieved in a batch reactor with a rotary agitator to provide mixing. An oscillatory flow offers a highly efficient alternative means of 'agitation'. We introduce an innovative Oscillatory Baffled Reactor (OBR) which consists of a reactor tank and oscillated 'donuts' shaped baffles. The oscillatory flow in the OBR produces well defined vortices as opposed to small-scale eddies in traditional batch crystallizers. Oscillatory flow generates tighter particle residence time distribution (RTD) as well as enhances mass and energy transfer. OBR also poses opportunities for continuous operations similar to MSMPR (mixed-suspension mixed-product removal). This study presents the evaluation of OBR performances of crystallization systems in terms of product quality for batch and continuous operations. We also explored control strategies to produce better quality crystalline drug substance.

10:05 AM **Mixing of Viscous, Non-Newtonian Fluids** (TueA3b)

Richard K. Grenville, Jason J. Giacomelli (Philadelphia Mixing Solutions Ltd.)

Reliable correlations have been developed for estimating blend times for Newtonian fluids in stirred tanks operating in the turbulent, transitional and laminar regimes. Most viscous fluids processed in the chemical industries exhibit non-Newtonian rheologies. Of these the vast majority are shear-thinning. This means that the apparent viscosity of the fluid will be low near the impeller, where velocity gradients are high, and high near the vessel wall where velocity gradients are low.

This presentation will discuss how to select the impeller type that is appropriate for a particular operating regime (Reynolds number). Then correlations for estimating blend times in Newtonian fluids will be discussed and how they can be modified to take account of non-Newtonian fluid behavior.

10:25 AM **Alternating Avalanches of Wetted Particles in Quasi-2D Heap Flow** (TueA3c)

John S. Hruska, Hongyi Xiao, Julio M. Ottino, Richard M. Lueptow, Paul B. Umbanhowar (Northwestern University)

Rotating and other axially asymmetric flows of dry sand poured on a heap have been observed previously. Here we describe analogous instabilities about the feed zone in heap flows of damp spherical glass particles and characterize the instability as a function of water content, particle size, and flow rate. In a quasi-two-dimensional bounded heap with a centrally located feed zone, the flow of spherical glass particles on the two sided heap bifurcates from symmetric steady flow to alternating avalanches down each side of the heap as the water content is increased. An intermediate regime exists where avalanches flow continuously down both sides of the heap simultaneously, but are out of phase. Alternating avalanches occur when as little as 0.01% of water by volume is added to 0.5 mm diameter particles, and the percentage of water required to trigger the transition increases with increasing particle diameter. Further increase in water content leads both to clumping and to a higher angle of repose for the avalanches. Based on our observations, we propose a mechanism for the bifurcation from steady symmetric flow to alternating avalanches related to the dependence of the angle of repose on water content. 3D heaps with and without a bounding wall show analogous behavior in the form of axially asymmetric flow including revolving rivers. Understanding such flow instabilities is important in silo filling and emptying, and other industrial applications. Funded by NSF Grant CBET-1511450 and Northwestern University.

10:45 AM **A Brownian Dynamics Study on Ferrofluids under Nonuniform Magnetic Fields using an Iterative Constraint Method to Satisfy Maxwell's Equations** (TueA3d)

Sean Dubina, Lewis Wedgewood (University of Illinois at Chicago)

Ferrofluids are steadily rising in applications across many fields, preferred for their ability to be remotely positioned and controlled via external magnetic fields. The response of particles in ferromagnetic clusters under uniformly applied magnetic fields has been reproduced using Brownian dynamics, Stokesian dynamics, and Monte Carlo methods. However, hardly any research has been developed to explore magnetophoresis, a migration phenomenon that ferroparticles experience in the presence of magnetic field gradients, especially at the particulate level. Moreover, prior ferrofluid modeling assumes that magnetization is a direct consequence of the magnetic field, a postulate that may be justifiable in dilute homogeneous solutions but invalid for dense suspensions or nonuniform magnetic fields. Therefore, a constraint method is developed to satisfy Maxwell's equations when a nonuniform magnetic field is implemented across a dense colloidal suspension in a heterogeneous Brownian dynamics model that examines the effects of ferromagnetic clusters amidst a mesoscale particle collection. The procedure ensures that essential laws of magnetostatics are met, namely Maxwell's equations. In conclusion, the resultant constraint model, employed with the Brownian dynamics technique, generates chain-like cluster formations, magnetic separation, and realistic ferrofluid behavior under a nonuniformly applied magnetic field while observing fundamental magnetostatic laws. Non-Newtonian fluid properties, aggregation activity, and separation results are compared to existing Brownian dynamics simulations and experimental data.

11:05 AM **A Universal Interpretation for Transient Nonlinear Rheology** (TueA3e)

Jiho Choi, Simon A. Rogers (University of Illinois at Urbana-Champaign)

A large number of soft material undergo strong and fast deformation in their formation, processing, transport, and use. Understanding the transient nonlinear rheology will lead to better energy efficiency and more accurate product formation with less material loss. However, no universal nonlinear rheological framework exists. This work addresses that need.

The most prevalent experimental method for understanding viscoelasticity is oscillation rheology, because large amplitude oscillatory shear (LAOS) makes it possible to study nonlinear rheology. Among analytic frameworks for LAOS, Fourier transform (FT) rheology [Wilhelm (2002)] is the standard method of analyzing nonlinear periodic signals to calculate their Fourier transform and quantify the harmonics higher than the fundamental. Despite FT rheology being the method of choice, there are serious issues surrounding its use such as a complete lack of physical interpretation for infinite odd harmonics. A possible solution is found in a recently-published technique based on differential geometry that is being referred to as the sequence of physical processes analysis. This work provides the clear link between the frameworks, providing, for the first time, a physical interpretation of all higher Fourier harmonics. In this work, it is shown how the SPP parameters are linked to the Fourier-based metrics and the other major metrics proposed in the literature. This makes possible to assign physical meaning to the higher harmonics not individually, but collectively, in non-trivial combinations. Specifically, the time-dependent dynamic moduli are shown to follow a well-defined path in elasticity-viscosity that traces out a deltoid shape with regard to asymptotic nonlinear regime with carrying instantaneous physical information at every single point. For nonlinear regime, this work suggests that a trajectory in two-dimensional parametric plot between dynamic viscous and elastic moduli, is formed by combination of deltoid and n-branched stars based on the fact that every n-th harmonic has perfect n-branched star.

Further, this research proves that the SPP approach encompasses other measures that are only defined at specific instances such as GM' and $\eta M'$ suggested by Ewoldt et al. (2008) and generalizes them to the entire period. Also, this study shows that the time average value of the SPP parameters over a period is identically equal to the first harmonic moduli which are generally regarded as representing the average energy dissipated and stored over a period. The ability to define time-dependent moduli allow us to unambiguously define a standard deviation from the mean over a period, allowing data from traditionally-performed strain amplitude sweeps to be enhanced significantly. Moreover, this research shows how the time-dependent SPP parameters can be obtained for responses to arbitrary time-dependent inputs. This includes deriving the SPP parameters for responses to arbitrary periodic driving functions, not just perfect sinusoids. These results will allow researchers to apply excitations that more closely match their processing or environmental conditions.

In contrast with existing approaches assigning physical explanation for each coefficient, this work combines the coefficients to form the time-dependent moduli of the SPP formalism. Three basic rheological models are investigated under the common sinusoidal strain input to demonstrate how the combination of the coefficients for the time-dependent moduli reduces the complexity of Fourier coefficients and shows suitable physical interpretations. Furthermore, analysis for fumed silica colloidal suspension as an experimental example is suggested.

Catalysis I

Tuesday, February 28, 2017 (Cardinal Room, **TueB1**)
Chair: *Feng Xu* (UOP/Honeywell)
Co-Chair: *Masoudeh Ahmadi* (University of Louisville)

2:00 PM **Durability Study of Electrocatalysts for Oxygen Reduction Reaction Using In Situ Quick Scanning Extended X-Ray Absorption Fine Structure** (TueB1a)
Thao Ngo, Hong Yang, (University of Illinois at Urbana-Champaign), *Chengjun Sun* (Argonne National Laboratory)

One major challenge hindering the large-scale utilization of high-performing polymer electrolyte membrane fuel cells (PEMFCs) is the durability of catalysts for the cathodic oxygen reduction reaction (ORR). In catalytic systems that shown enhanced activity such as faceted platinum–transition metal (Pt–M) bimetallic catalysts (M are Fe, Co, Ni and Cu), continuous leaching of the non-noble, more reactive metals during long–term stability tests contributes to degradation in mass activity. A previous study by the Yang group at the University of Illinois at Urbana-Champaign showed that carbon-supported truncated octahedral Pt_3Ni catalyst lost 21% of its initial electrochemical surface area (ECSA) and 40% of its mass current density (from 0.55 to 0.33 A/mgPt) after 30,000 potential cycles under acidic environment. This compares to a 44% loss in ECSA and 41% loss in mass-current density (from 0.16 to 0.093 A/mgPt) of commercial catalysts. To control metal leaching and achieve improved catalytic performance and durability, it is essential to understand the underlying mechanism and kinetics of metal leaching in faceted Pt bimetallic catalysts. In this study, in situ quick scanning extended X-ray absorption fine structure (QEXAFS) and X-ray absorption near-edge spectroscopy (XANES) is used to probe the leaching of Ni from Pt-Ni nanocatalysts in real time, providing information on the compositional change of the catalysts as they are being used.

2:20 PM **A Mechanistic Study of the Validity of Using Hydroxyl Radical Probes to Characterize Electrochemical Advanced Oxidation Processes** (TueB1b)
Yin Jing, Brian P Chaplin (University of Illinois at Chicago)

The detection of hydroxyl radical (OH•) are typically accomplished by using reactive probe molecules, but prior studies have not thoroughly investigated the suitability of these probes in electrochemical advanced oxidation processes (EAOPs), due to the neglect of alternative reaction mechanisms. In this study, we investigated the suitability of four OH• probes, coumarin, p-chlorobenzoic acid, terephthalic acid, and p-benzoquinone for use in EAOPs. Experimental results indicated that both coumarin and p-chlorobenzoic acid are oxidized via direct electron transfer (DET), while p-benzoquinone and terephthalic acid are not. Coumarin oxidation to form the OH• adduct product 7-hydroxycoumarin was found at anodic potentials lower than that necessary for OH• formation. Density functional theory (DFT) simulations found a thermodynamically favorable and non-OH• mediated pathway for 7-hydroxycoumarin formation, which is activationless at anodic potentials > 2.10 V/SHE. DFT simulations also provided estimates of Eo values for a series of OH• probe compounds, which agreed with select voltammetry results. Results of this study should guide the proper selection of OH• probe compounds for the characterization of electrochemical and catalytic systems.

2:40 PM **Oxidative Dehydrogenation of Ethane to Ethylene over a novel perovskite** (TueB1c)
Maasoomeh Jafari, Jason Trembly (Ohio University)

Ethane is an important feedstock for the petrochemical industry and is used to produce ethylene, a key building block for many important chemicals. Development of unconventional gas resources has increased U.S. ethane production by 50 percent over the past eight years, with significant product growth still expected. Industry has responded increasing current ethylene plant production, pipeline, and export capacities. However, these expansions will not be sufficient to stop ethane rejection or re-injection. To address the overabundance of ethane, additional ethane conversion capacity is needed.

Conventional ethylene production completed via steam cracking of ethane, which is thermodynamically limited and highly energy intensive, results in significant CO_2 and criteria pollutant emissions while being highly capital intensive. Due to these issues, only a few new steam cracking facilities are being considered. Oxidative dehydrogenation (ODH) of ethane is an attractive alternative ethylene production technique, as the process is exothermic and is not thermodynamically limited. New chemical looping-based ODH processes show even greater promise, as they do not require air separation. However, even these newest ODH concepts are capital intensive and require ethane to be first separated from its natural gas constituents.

To address these issues, Ohio University (OHIO) is developing a modular electrogenerative ODH concept allowing for ethylene production at the well pad site without gas separation or large capital costs. The key to this process is a catalyst with suitable ODH activity and mixed ionic/electronic conductivity. Many researchers have been working towards the development of such materials and among them perovskite structured oxides show great promise. OHIO has been pursuing the development of a new perovskite-based material synthesized using a modified Pechini method. In this presentation, results from these studies will be provided including x-ray diffraction and scanning electron microscopy analyses, ionic and electronic conductivity and ethane conversion and product selectivitiy with temperature.

3:00 PM **Composite Metal Oxide/Zeolite Monoliths for Catalysts in Alcohols Dehydrations** (TueB1d)
Xin Li, Fateme Rezaei, Ali Rownaghi (Missouri University of Science and Technology)

Structured catalysts with elaborate structure, special geometry and tunable porosity offer an excellent gas-solid contacting strategy for development of practical and scalable chemical transformation technologies. In this study, the fabrication of three-dimensional (3D)-printed nanoporous zeolite monoliths of HZSM-5, HY and SAPO-34 with novel structures and their use in alcohols dehydration reactions were studied. The physical and structural properties of these printed composite monoliths are evaluated and compared with their powder counterparts. Here, we will present a systematic study of 3D-printed nanoporous zeolites catalyst preparation and testing for alcohol dehydration applications. These novel structures are expected to circumvent the drawbacks of packed bed catalyst such as high pressure drop, and heat and mass transfer limitations. More precise modification in the design of 3D printed composite zeolites can be accomplished through the use of zeolite growth modifiers and metal coating. The effect of these modification routes on catalytic performance of 3D-printed monolithic catalysts are investigated. Fabrication of catalysts with the 3D printing technique is proven to be promising due to its material-diversity, facileness and cost-effectiveness.

3:20 PM **The Effects of Zr Promotion on Co Dehydrogenation Catalysts** (TueB1e)
Yiqing Zhao, Adam S. Hock (Illinois Institute of Technology), *Hyuntae Sohn, Massimiliano Delferro* (Argonne National Laboratory)

Zirconium was found to promote the rate and improve the selectivity of our group's previously reported Co/SiO2 catalyst for propane dehydrogenation. The Co/Zr/SiO2 material exhibited high propene selectivity which can reach up to 98% for catalytic propane dehydrogenation at 550 ℃ with stable catalytic activity. The catalyst was characterized by transmission electron microscopy and X-ray near-edge and extended absorption fine structure of the as-synthesized material and under reaction conditions. Previous calculations found that weaker catalyst-oxygen bonds led to facile heterolytic cleavage and we hypothesize that the improved dehydrogenation activity is due to the ease of heterolytic cleavage of the propane C-H bond in the rate-determining step. This catalyst shows that rational catalyst design principles can be applied in heterogeneous systems using homogeneous catalyst design principles.

<u>Process Safety I</u>

Tuesday, February 28, 2017 (White Oak, **<u>TueB2</u>**)
Chair: *Scott M. Wozniak* (UOP/Honeywell)
Co-Chair: *Sonny Sachdeva* (PSRG)

2:00 PM **Don't Buy That New Building!** (TueB2a)
Ernesto Gasulla (Baker Risk Engineering and Risk Consultants)

Analysis of explosion hazards in petrochemical plants often results in unacceptable personnel risks for occupied buildings. After all process safety risk mitigation measures have been evaluated, risk might still be above the tolerable threshold, which may lead to the conclusion that the plant needs a new building. However, lack of real estate, infrastructure and utilities relocation costs (particularly for control buildings) and preference of the personnel working in those buildings make that a difficult and expensive decision. There is an alternative: in most practical cases, an existing building can be retrofitted to achieve an acceptable explosion risk level, usually without interrupting work and with minimal –if any- utility relocation costs. This presentation will discuss explosion retrofit strategies for different building types commonly found in petrochemical plants, including case studies.

2:20 PM **Why Risk It?: The Usage and Pitfalls of Risk Based Criteria** (TueB2b)
Ryan Terry, Charles King (PSRG)

There is a broad movement today for companies to adopt risk based criteria for a variety of process safety applications. Risk Based Facility Siting Studies, QRA and LOPA are several of the most prominent methodologies currently in use that employ some variety of risk based approach to safety. This approach can make sense, and can allow for a more detailed examination of site hazards. It can also create new issues with methodology and implementation that at best complicate the study, creating administrative backlog and scheduling issues, and at worst prevent sites from considering all of the potential onsite hazards. The focus of this presentation is to discuss the potential issues that arise with risk based criteria, and to provide guidance on if/when a risk based criteria makes sense and how to properly implement one within a company or facility.

2:40 PM **Combining Traditional UOP HAZOP/PHA Analysis with Dynamic Simulation A New Process Safety / Risk Assessment Tool** (TueB2c)
Scott M. Wozniak (UOP/Honeywell)

There is a clear link between safety and reliability in process design and operation. Traditional UOP HAZOP analysis identifies potential operational failures and weak points in a process design; evaluates risks introduced by them and develops effective risk reduction strategies before a customer takes delivery of a UOP Schedule A Process Design.

This paper shows how our current UOP HAZOP methodology is supported by dynamic simulation and modeling techniques. By leveraging this process technology, UOP can now deliver more robust HAZOP studies by integrating our current UOP Process Technology library of UNISIM flowsheet templates in all phases of the HAZOP work process. We will show how dynamic simulation can determine consequences of deviations from normal design exactly and how this tool can potentially identify new unknown hazards and safety issues.

3:00 PM **Evaluating Fire Hazards in Oxygen Enriched Atmospheres** (TueB2d)
Sean J. Dee (Exponent)

The fire triangle outlines the three necessary components for a fire: fuel, oxygen, and heat. Oxygen may appear the most benign from a fire safety standpoint because it is a non-flammable gas. However, the flammability of materials and their susceptibility to ignition can change dramatically if the concentration of oxygen is increased above ambient levels. The flammability hazards associated with oxygen enriched atmospheres (OEAs) impact several industries including chemical processing, industrial gas supply, aerospace, and medical. In this presentation, an overview of the fire hazards associated with OEAs will be discussed. The influence of OEAs on both metal and non-metal material flammability and several ignition mechanisms will be reviewed. Safety standards and industry best practices will also be discussed for mitigating the fire hazards in oxygen enriched atmospheres. Finally, a cast study will be presented to demonstrate the concepts related to fire hazards in oxygen-enriched atmospheres.

3:20 PM **Analysis of Refinery Pressure Vessels to Prevent Brittle Fracture** (TueB2e)
Jerry Wilks (CITGO Petroleum Inc.)
Brittle fracture of steels first became a recognized significant industrial problem during World War II when a series of ships experienced brittle fracture while in service in northern seas. Investigation of those ship failures and subsequent failures in other industries led to the adoption of modern fracture mechanics in engineering codes, standards, and government guidelines throughout the world. In the Oil Industry much of the equipment operates at high enough temperatures to avoid brittle fracture during typical operations. However, there are start-up and shut down situations that subject pressure vessels to combinations of stress and low temperature that could lead to brittle fracture. In an effort to minimize the time required for unit start-up and shut down, many refinery pressure vessels are being analyzed today to determine the minimum temperature over a range of pressures. The results of brittle fracture analyses of refinery pressure vessels are frequently presented in the form of "safe pressurization curves." These are graphs that show the temperature-pressure combinations where there is a risk of brittle fracture for each vessel on the unit. These curves make it possible to optimize the unit start up and shut down while minimizing the risk of brittle fracture. Also, after making repairs refinery pressure vessels are frequently hydrotested, and this subjects the vessel to higher than normal pressure while at low temperature. This paper provides several examples of analysis of refinery pressure vessels including codes and standards used for brittle fracture analyses. It also provides examples that show the effects of hydrogen charging of steel and examples of the brittle fracture risks that occur during hydrotesting.

<u>Fluid Dynamics and Transport Phenomena II</u>
Tuesday, February 28, 2017 (Illinois C, **<u>TueB3</u>**)
Chair: *Raj Venuturumilli* (BP)
Co-Chair: *Abdelaziz Lafi Khlaifat* (Abu Dhabi Polytechnic)
2:00 PM **Optimization of Binder Addition for Spherical Agglomeration in Oscillatory Baffled Crystallizers** (TueB3a)
Kanjakha Pal, Joseph A. Oliva, Ramon Peña, Zoltan K. Nagy (Purdue University), *Christopher L. Burcham*, *Daniel J. Jarmer* (Eli Lilly and Company)
Spherical Agglomeration is a new Process Intensification (PI) Technology which promises significant reduction of manufacturing costs in the pharmaceutical industry. Spherical Agglomeration combines crystallization and granulation unit operations in a combined unit operation and thereby eliminates a few process steps in pharmaceutical manufacturing hence reducing cost. Although there have been improvements in continuous spherical agglomeration using Mixed Suspension Mixed Product Removal Crystallizers (MSMPR), controlling Agglomerate Size Distribution(ASD) using traditional MSMPRs has been proven to be very difficult. Oscillatory Baffled Crystallizer (OBC) has emerged as a promising alternative to traditional MSMPRs for continuous crystallization processes. In OBCs, there is oscillatory motion superimposed on plug flow which gives a unique combination of the advantages obtained in plug flow systems and advantages from Mixed Suspension systems. Binder addition in such an Oscillatory Baffled System has been traditionally done in one injection port of the Oscillatory Baffled Crystallizer. In this work a non-linear optimization of the binder addition profile in an Oscillatory Baffled Crystallizer has been carried out and it was seen that the final product properties of the agglomerates obtained from the optimum binder addition profile were better than the final product properties of the agglomerates obtained by using a constant binder addition profile.

2:20 PM **Visualizations of Local Hydrodynamics for Airlift Reactor: 3D Velocity Domain** (TueB3b)
Laith Salim Sabri, Abbas Sultan (Missouri University of Science and Technology)
The airlift reactor are extensively used in chemical and biochemical industries. Where perfect mixing and ideal mass transfer are importance. The scope of this work, airlift reactor with internal (split plate) was used for air-water system. The local hydrodynamics can considerably affect the reactor conduct. Due to the local hydrodynamics parameters are the main factor for multiphase reactor design. Consequently, effective reactor design and successful scale-up require a suitable understanding of the local hydrodynamics for multiphase flow. Unfortunately, these parameters need to be further developed and evaluated to account of 3D flow field in each position inside the reactor which is unclear yet. Therefore, the advanced non-invasive measurement techniques Radioactive Particle Tracking (RPT) has utilized to investigate flow features in the 5.5-inch (0.14m) inner diameter Plexiglas split airlift reactor.

For present study, quantifies of the flow characterization in the time series of lagrangian tracer particle trajectory are available for fluctuating liquid velocity fields at various superficial gas velocities (1 and 3 cm/sec). As a result, the experimental results provide benchmark data for simulation, design, scale-up, and performance calculation of split reactor. The experimental results and conclusions will present at the conference.

2:40 PM **4-phase Flow Model for Natural Gas Production from an Unconsolidated Hydrate Reservoir** (TueB3c)
Deniz Hinz (Illinois Tech)
Natural gas from hydrates is a promising source of energy as we transition to a sustainable energy society. The dissociation of solid hydrate in the reservoir into gas and water results in a rapid and dramatic reduction in strength of the sediment matrix, such that the sand behaves like unconsolidated sediment. We have developed a CFD model to simulate the hydrate dissociation and four phase production of gas, water, hydrate and sand from a methane hydrate reservoir.

3:00 PM **Size Segregation in Sheared 3D Granular Flows** (TueB3d)
Adithya Shankar, Alex M. Fry, Paul B. Umbanhowar, Julio M. Ottino, Richard M. Lueptow (Northwestern University)
Size segregation of granular materials is a commonly encountered problem in industry. Many approaches have been taken to model the effects of segregation in granular flows; however, the underlying mechanism behind the phenomenon is still not well understood. In this study, we perform a series of 3D Discrete Element Method (DEM) simulations to measure the segregation

force on a single large particle in a granular shear flow to explore the underlying mechanism driving size segregation. To measure segregation forces, the large particle is tethered by a spring in the vertical direction in a shearing bed of small particles. We characterize the scaled segregation force (relative to buoyancy) on the large particle as a function of particle size ratio and flow kinematics. As found previously for 2D simulation of disks, the scaled segregation force exhibits a maximum at a size ratio of 2. However, scaled segregation force acting on spherical particles in 3D is approximately twice as large as the corresponding forces on disks in 2D.

3:20 PM **Momentum Transfer with Co-axially Placed Twisted-tape Disc Assembly as Turbulence Promoter in Circular Conduit** (TueB3e)
K.Siva Kumar (Samara University), *V.Nageswara Rao, M.Gangadhar* (Andhra University)
Studies on the effect of coaxially placed entry region twisted tape-disc assembly as turbulence promoter on momentum transfer rates in forced convection flow of electrolyte were conducted. The study covered a wide range of geometric parameters such as pitch of the tape (TP), length of the tape ((TL), width of the tape (TW), diameter of the disc (Dd), and tape-disc distance (h). The results revealed that the friction factor increased with increase in diameter of the disc (Dd), length of the tape (TL), width of the tape (TW) and decreased with increase in pitch of the tape (TP) and tape-disc distance (h). Within the range of variables covered, the increase in friction factors due to the presence of the promoter assembly was significant. At the velocity of 0.224m/s, while for the maximum augmented promoter assembly the increase was 28.5 times more than the smooth tube, while for the minimum augmented promoter assembly the increase over the smooth tube was 27.2 times. Momentum transfer rates were analyzed with momentum transfer roughness function R(h+) and roughness Reynolds number (Re+).

Electrochemical Energy Storage
Tuesday, February 28, 2017 (Illinois B, **TueB4**)
Chair: *Jie Xu* (University of Illinois at Chicago)
Co-Chair: *Bader Jarai* (AllCell Technologies)

2:00 PM **Material Design of Low-Dimensional Carbon Nanomaterials for Rapid Energy Storage** (TueB4a)
Alex Pak (University of Chicago), *Gyeong S. Hwang* (University of Texas at Austin)
Low-dimensional carbon materials, such as graphene and nanoporous carbon, have become increasingly explored for use as electrodes in electrochemical double layer capacitors, owing to their high specific and volumetric surface area and good electrical conductivity; according to classical double layer theory, the capacitance is proportional to surface area. However, experiments report a wide and unexpected spectrum of capacitances, including both anomalously small and large values, thereby highlighting a need for an improved understanding of the fundamental charge storage mechanisms. As the performance of these devices is primarily related to the evolution of the electrode-electrolyte interfacial microstructure, atomistic insights from molecular simulations can help provide the guidance needed to design materials with better and more reliable performance. To this end, we present an overview of our work toward this goal which leverages a strategy that combines classical molecular dynamics with ab-initio density functional theory. First, we describe a concept known as the quantum (or electrode) capacitance that becomes relevant due to low-dimensionality. Second, we explore non-equilibrium dynamics associated with extreme confinement within subnanometer pores. We will discuss the relative influence of these factors on graphene-based nanomaterials and nanoporous carbons and conclude with strategies to utilize these insights for the improved design of electrode materials for supercapacitors.

2:20 PM **A Rechargeable Membraneless Enzyamtic Fuel Cell for use as an Implantable Device** (TueB4b)
Alireza Ahmadianyazdi, Roberto Preite, Jie Xu (University of Illinois at Chicago), *Ross D. Milton*, *David P. Hickey, Shelley D. Minteer* (University of Utah)
Enzymatic fuel cells can be implanted in living organisms to exploit the chemical energy stored in physiological fluids. Generally, the electron donors such as sugars are ubiquitous in in vivo environment, while electron acceptors such as oxygen are limited due to many factors including solubility, temperature, and pressure. The wide range of solid-state cathodes, however, may replace the need for oxygen breathing electrodes, and serve in enzymatic biobatteries for implantable devices. Here, we have fabricated a glucose biobattery suitable for in vivo environment with employing a glucose oxidase (GOx) anode coupled to solid-state Prussian Blue (PB) thin-film cathode. Prussian Blue is a non-toxic material that can be produced in large scale by a low-cost synthesis route. More importantly, its electrochemistry enables fast regeneration if used in a secondary cell. This novel biobattery can effectively operate in a membraneless architecture, as Prussian Blue can reduce the peroxide produced by some oxidase enzymes. The resulting biobattery has an open circuit voltage of 0.45 V, and it delivers a maximum power and current density of 44 μW/cm2 and 0.9 mA/cm2, respectively, which is ca. 37% and 180% higher than an equivalent enzymatic fuel cell equipped with a bilirubin oxidase cathode. Moreover, the biobattery demonstrated a stable performance over 20 cycles of charging and discharging periods with only ca. 3% loss of operating voltage.

2:40 PM **Development of Advanced MnO2 Nanostructures for Highly Rechargeable Cathodes; Bi Doping and Electrochemical Performance in Aqueous Electrolyte** (TueB4c)
Elahe Moazzen (Illinois Tech)
Manganese (IV) oxide (MnO2) has attracted significant attention as a cathode material in battery industry due to its high theoretical capacity (308 mAh/g), low cost and low toxicity. Although this material has been used in primary aqueous and secondary non-aqueous batteries, the application in rechargeable aqueous batteries is facing some big challenges such as capacity fading and cycle life. MnO2 can exist in several structural forms: alpha (α-MnO2), beta (β-MnO2, pyrolusite), ramsdellite (R-MnO2), gamma (γ-MnO2), delta (δ-MnO2, Birnessite) and epsilon (ε-MnO2, Akhtenskite), where MnO6 octahedral units are linked together in various ways through corner- or edge-sharing to form layered or tunneled structures. Among these structural phases, ε- and γ-MnO2 are the most electrochemically active ones. Therefore, any synthesis rout targets these structures and tries to eliminate others. Electrochemical performance of this cathode material

strongly depends on the morphology and crystal structural composition. Therefore, the first part of this study reports on an oxidation methodology that we developed in the past year to produce MnO_2 nanostructures with a precise and systematic control on the morphology and phase composition of the products. We managed to synthesize MnO_2 nanoplatelets with uniform distribution in size (200x20 nm) and shape and high ε-MnO_2 content (76%). The product showed an exceptional rechargeable electrochemical performance (galvanostatic cycling) in LiOH electrolyte (~210 at 50th cycle). This is the first time that MnO_2 cathode rechargeable cycling in an aqueous electrolyte is reported with no fading in discharge capacity. This phenomenon can be contributed to the contribution of the factors including nano size and the unique morphology of the particles, which facilitate Li ions intercalation by increasing the ions capacity and availability and reducing the diffusion baths, and phase composition of the nanoparticles (24 wt. % R-MnO_2:76 wt. % ε-MnO_2). The second part of the study presents Bi doping of the nanoparticles and its effects on the capacity, cyclibility, discharge potential and cycle life of the MnO_2 nanoparticles.

3:00 PM **Thermal Runaway Mitigation in Lithium-ion Battery Pack using Phase Change Composite Material** (TueB4d)
Siddique Khateeb, Stephen Wilke, Gregory Wilk, Said Al-Hallaj (AllCell Technologies)

Thermal Management of Lithium-ion batteries is very crucial for normal operating conditions and during unexpected battery abuse conditions that leads to battery thermal runaway. Current state-of-art strategies such as air-cooling, liquid cooling methods are most widely in electric vehicles but they have inherent disadvantages such as complex system architecture, large parasitic power consumption, additional weight and volume. Such systems rely on dedicated power system to be operational and cannot function when vehicle is turned OFF. Also, such systems have not been designed to dissipate large amount of heat during the event of thermal runaway and prevent thermal runaway propagation. Recently, passive thermal management systems using a phase change composite (PCC) material has been successfully demonstrated for light electric vehicles and other light duty applications.

PCC material based thermal management system does not rely on external power systems and are easily integrated inside a battery pack. PCC material is made up of 22% (by weight) high thermal conductivity graphite and 78% (by weight) PCM inside graphite pores. PCC material maintains the battery pack at optimal temperature by utilizing graphite's thermal conductivity to dissipate heat faster that is absorbed as latent heat by PCM. Apart from maintaining battery pack at optimal temperature, the PCC material can dissipate large amount of heat in the event of a thermal abuse event that causes a cell to release large quantity of exothermic heat. In this research work, thermal abuse testing of lithium-ion battery pack is performed using different thermal management strategies and results are reported. Thermal abuse testing of a lithium-ion battery pack is performed using a nail penetration test on a single cell and evaluating the thermal runaway propagation effects to neighboring cells. The role of thermal conductivity, latent heat storage capacity is evaluated by testing a battery pack with four different strategies namely – air only, PCM only, graphite only and PCC (PCM+Graphite). The experimental results showed that except battery pack with PCC material, all packs had severe thermal runaway propagation effects resulting in fire and severe damage to battery pack was observed after tear-down analysis. The results clearly suggest that PCC material could prevent thermal runaway propagation in a battery pack because of the combination of high thermal conductivity graphite that dissipated the heat away from trigger cell and presence of PCM in graphite pores that absorbed large quantity of heat released from the trigger cell and prevented over-heating.

3:20 PM **Life Cycle Analysis of the Production of Rare Earth Metals and Alloys via Electrowinning** (TueB4e)
Ehsan Vahidi, Fu Zhao (Purdue University)

Due to the importance of Rare Earth Elements (REEs) in many high-tech and clean energy applications, they have received increased attention in recent years. Although production pathway of REEs is known to be environmental destructive, very limited Life Cycle Assessment (LCA) investigations have yet been conducted. This is particularly true for the electrolysis of the rare earth oxides in a medium comprising lithium fluoride and rare earth fluorides, a key step in the high-purity rare earth metals production pathway. In this study, a comparative LCA is carried out on different electrowinning processes in China using graphite and tungsten as anode and cathode, respectively. The material and energy flow data were based on production information collected from three electrowinning facilities in China. In combination with mass/energy balance and stoichiometry, the life cycle inventories were developed using SimaPro 8 software and Ecoinvent 3 database and the life cycle impact was evaluated by TRACI. LCA results were utilized to determine and quantify environmental hotspots of the electrowinning process. Finally, challenges and opportunities for improved environmental performance of the rare earths electrowinning process were discussed.

Catalysis II

Tuesday, February 28, 2017 (Cardinal Room, **TueC1**)
Chair: *Belma Demirel* (Guidepoint)
Co-Chair: *Wan-Ting Chen* (University of Illinois at Urbana-Champaign)

4:00 PM **Oxygen Evolution Reaction Kinetics on Porous $LaCoO_3$ Perovskite** (TueC1a)
Jaemin Kim, Pei-Chieh Shih, Xuxia Chen, Boquan Li, Hong Yang (University of Illinois at Urbana-Champaign)

Extensive research efforts have been placed on the study of water electrolysis for sustainable energy production. Nevertheless, effective hydrogen production is hampered by sluggish oxygen evolution reaction (OER). Although acidic media is preferred due to high ionic conductivity and fewer side reactions during OER process, feasible oxygen evolution can be performed in alkaline media with cost-effective manners. Among the first-transition metal, cobalt- and nickel-based oxides are known to be good OER catalysts. More specifically, $LaCoO_3$ is known as one of the best OER catalysts in alkaline media, but it delivers low specific activity mainly due to large grain size. In this talk, I will present a process for making nanoporous structure of $LaCoO_3$ at low temperature. This porous catalyst showed significantly enhanced OER mass activity arise from the increased surface area because of reduced grain size and porous morphology. More importantly, this nanoporous structure affects the OER kinetics. The derived kinetic parameters from our experimental measurement, which include exchange current densities, transfer coefficients and Tafel slopes, strongly support the fast OER kinetics on the porous structures. Our findings further suggest a new design strategy for the ternary metal oxides electrocatlaysts in oxygen involved reaction chemistry.

4:20 PM **Influence of Self-Assembling Redox Mediators on Charge Transfer at Hydrophobic Electrodes** (TueC1b)
Timothy J. (Tim) Smith, Nicholas L. Abbott, Chenxuan Wang (University of Wisconsin - Madison)
We report that reversible self-assembly of aqueous solutions of amphiphilic redox-mediators at chemically functionalized electrodes can be exploited to influence interfacial charge transfer processes in potentially useful ways. Specifically, we employed (11-ferrocenylundecyl)-trimethylammonium bromide (FTMA) as a model self-assembling redox mediator and alkanethiol-modified gold films as hydrophobic electrodes. By performing cyclic voltammetry (CV, 10 mV/s) in aqueous solutions containing FTMA above its critical micellar concentration (CMC), we measured anodic (Ia) and cathodic (Ic) peak current densities of 18 ± 3 μA/cm2 and 1.1 ± 0.1 μA/cm2, respectively, revealing substantial current rectification (Ia/Ic= 17) at the hydrophobic electrodes. In contrast, hydroxymethyl ferrocene (a non-self-assembling redox mediator) at hydrophobic electrodes and FTMA at bare gold electrodes yielded relatively low levels of rectification (Ia/Ic= 1.7 and 2.3, respectively). Scan-rate dependent measurements revealed Ia of FTMA to arise largely from diffusion of FTMA from bulk solution to the hydrophobic electrode whereas Ic was dominated by adsorbed FTMA, leading to the proposal that current rectification observed with FTMA arises from interfacial assemblies of reduced FTMA that block access of oxidized FTMA to the hydrophobic electrode. Support for this proposal was obtained by using atomic force microscopy and quartz crystal microbalance measurements to confirm the existence of interfacial assemblies of reduced FTMA (1.56 ± 0.2 molecules/nm2). Additional CV of a mixed surfactant system containing FTMA and dodecyltrimethylammonium bromide (DTAB) revealed that interfacial assemblies of DTAB also block access of oxidized FTMA to hydrophobic electrodes; this system exhibited Ia/Ic>80. These results and others reported in this paper suggest that current rectification occurs in this system because oxidized FTMA does not mix with interfacial assemblies of reduced FTMA or DTAB that form at hydrophobic electrodes. More broadly, these results show that self-assembling redox mediators offer the basis of new approaches to controlling charge transfer at electrode/solution interfaces.

4:40 PM **Fluorination of Boron-doped Diamond Film Electrodes for Minimization of Perchlorate Formation** (TueC1c)
Pralay Gayen, Brian P Chaplin (University of Illinois at Chicago)
This research investigated the effects of surface fluorination on both rates of organic compound oxidation (phenol, terephthalic acid (TA)) and perchlorate (ClO4-) formation at boron-doped diamond (BDD) film anodes at 22o C. Different fluorination methods (plasma assisted fluorination, non-aqueous perfluorooctanoic acid (PFOA) oxidation and silanization) have been used to incorporate –CnF2n+1 (0 ≤ n ≤ 8) moieties on the BDD surface. X-ray photoelectron spectroscopy measurements determined that these various fluorine functional groups were incorporated by electrochemical oxidation of non-aqueous (in formic acid) perfluorooctanoic acid solutions, radio frequency (RF) plasma with H2/CF4 gas, and silanization with aliphatic (1H,1H,2H,2H perfluorodecyltrichlorosilane) and aromatic (trimethyl(pentafluorophenyl)silane) precursors. Batch oxidation experiments revealed that ClO4- formation via the oxidation of ClO3- was highly variable with different surface modification methods while organic compound oxidation rates were not significantly affected. The ClO4- formation was not detected with the aliphatic silanized electrode (<0.12 μmoles m-2 min-1) while organic oxidation was not significantly affected (phenol: 60% and TA: 58% decrease). The non-aqueous (in formic acid) perfluorooctanoic acid oxidation modified electrode showed decrease in ClO4- formation (65%) but the organic oxidation increased (phenol: 26% and TA: 55%) due to enhanced hydrophobic interaction. Fe(CN)63-/4- and Fe3+/2+ redox couples using cyclic voltammetry and electrochemical impedance spectroscopy indicated that ClO4- formation was below the detection limit (<0.12 μmoles m-2 min-1) on the aliphatic silanized electrode was due to steric hindrance between the fluorinated chain and ClO3- and hydrophobicity of the fluorinated electrode rather than electrostatic interactions between the negative ClO3- anions and negative F dipoles. This is confirmed by almost same perchlorate formation before and after plasma fluorination and aromatic silanization due to short chain length of fluorinated groups. The aliphatic silanized electrode also showed very high stability under OH● production showing perchlorate formation below the detection limit (<0.12 μmoles m-2 min-1) up to 10th cycle and showed almost 90% decrease on ClO4- formation thereafter.

5:00 PM **The Effect of Support Morphology on Co/CeO2 Catalysts for the Reduction of NO by CO** (TueC1d)
Louisa Savereide, Justin M. Notestein (Northwestern University)
Developing non-precious metal catalysts for the reduction of nitrogen oxides is an important goal for reducing toxic automotive emissions. Transmission metal oxides supported on ceria have shown promising activity for reducing NO. Incipient wetness impregnation (IWI) is a simple, scalable technique for producing these types of catalysts; however, IWI leads to a variety of types of cobalt oxide surface species that cannot be easily controlled. Different exposed planes of ceria stabilize cobalt oxide in different ways, and may provide a handle for understanding the relationship between types of cobalt oxide species and catalyst activity.

In this study, cobalt (II) nitrate hexahydrate was deposited on ceria of different morphologies via IWI. Materials were tested for the reduction of NO by CO in a flow reactor at atmospheric pressure with temperatures ranging from 150-450 oC. Catalysts were characterized with diffuse reflectance ultra violet spectroscopy (DRUV-vis), Raman spectroscopy, carbon monoxide and hydrogen temperature programed reduction (CO-TPR), powder x-ray diffraction (XRD), and x-ray absorption spectroscopy (XAS).

5:20 PM **Development of 3D-Printed Monolithic Adsorbents and Evaluation of CO2 Adsorption Performance** (TueC1e)
Harshul Thakkar, Harshul Thakkar, Stephen Eastman, Amit Hajari, Ali Rownaghi, Fateme Rezaei (Missouri University of Science and Technology)

Structured adsorbents, especially in the form of monolithic contactors, offer an excellent gas−solid contacting strategy for the development of practical and scalable CO2 capture technologies. In this study, the fabrication of three dimensional (3D)-printed zeolite and aminosilica monoliths with novel structures and their use in CO2 capture were investigated. The physical and structural properties of these printed monoliths were evaluated and compared with their powder counterparts. For each class of material, the weight fractions of binder, co-binder and plasticizer were varied to optimize the adsorption performance and mechanical stability of the 3D-printed monoliths. Our results indicated that 3D-printed monoliths with high adsorbent loadings as high as 90 wt% exhibit adsorption uptake that is comparable to that of powder sorbents. The dynamic CO2 /N2 breakthrough experiments showed relatively fast dynamics for monolithic structures. Moreover, the printed zeolite monoliths showed reasonably good mechanical stability that can eventually prevent attrition and dusting issues commonly encountered in traditional pellets and beads packing systems. The 3D printing technique offers an alternative, cost-effective, and facile approach to fabricate structured adsorbents with tunable structural, chemical, and mechanical properties for use in gas separation processes.

<u>Process Safety II</u>

Tuesday, February 28, 2017 (White Oak, **<u>TueC2</u>**)
Chair: *Brenton Cox* (Exponent)
Co-Chair: *Brian Slusar* (BP)

4:00 PM **Maintaining a Positive Process Safety Culture** (TueC2a)
Sonny Sachdeva (PSRG)

Most facilities strive for occupational health and safety excellence but, although it appears they have excellent safety programs in place, incidents still occur. During this presentation, PSRG will explore a key factor to achieving and maintaining safe operations – a heathy Process Safety Culture. The presentation will discuss the features of best-in-class safety culture and how to develop and maintain it. The authors will discuss the role of management, and importance of resource allocation, communication, training, and continuous improvement to develop and implement a sound culture of safety. This will help the audience to benchmark their safety culture and in exploring room for improvement in their current safety programs.

4:20 PM **Near Misses and Where to (Not) Find Them** (TueC2b)
Mike Moosemiller (Baker Risk Engineering and Risk Consultants)

Fortunately, the focus on safe behaviors, hazard recognition, and risk management has greatly improved over the past few decades. However, in the early days of the author’s careers, there wasn’t the same level of safety awareness - and much more risk-taking behavior. In this paper, the author recounts events in which he (and others) were ignorant, careless, or actively put themselves in dangerous situations. These poor choices could have, or did actually result in, chemical exposures, fall hazards, overpressure events, and process upsets. The author describes the circumstances leading to the decisions to take personal risks, what happened (and what could have happened), and the consequences resulting from those poor choices. These same events could happen today to inexperienced (or even experienced) engineers, and it is hoped that the lessons learned by the author will prevent others from putting themselves in risky situations.

4:40 PM **Emergency Isolation Valves (EIVs) and its impact on Process Safety** (TueC2c)
Scott M. Wozniak (UOP/Honeywell)

An Emergency Isolation Valves (EIV) is used as a means of isolating flammable or toxic substances in the event of a leak or fire. The installation, and use, of EIV's in many hydrocarbon services will significantly reduce the potential of fire and explosion damages caused by loss of hydrocarbon containment situations; and a general improvement in overall plant safety for both capital assets, and operating / maintenance personnel. In Hydrocarbon, and / or toxic services; EIV's will serve to mitigate the potential of significant environmental releases.

This paper shows realistic design issues relevant to the installations of EIVs. The items to be covered include the code basis of EIV's (API RP-553, NFPA 58 specific requirements for LPG service), the types of valves to be used; the selection of manual or automatic valve actuation; guidelines for determining if EIV's are recommended based on equipment services, and hydrocarbon inventories; general installation requirements; and integration with other safety instrumented systems within the processing unit.

5:00 PM **Hazardous Area Electrical Classification/Zoning and its Role in a Process Safety Program** (TueC2d)
Stephen Garner, Justin Bishop, Jay Prigmore, Brenton Cox (Exponent)

Hazardous area electrical classification/zoning, as it relates to electrical equipment, is a systematic method of sub-dividing, three dimensionally, a facility into areas/zones of different categories according to the probability of occurrence of an explosive atmosphere. There are numerous national and international standards and directives governing area classification/zoning such as BSI, HSE (DSEAR-2002), NFPA, IEC, CEN, and CENELEC (ATEX118a directive). While regulatory compliance during the design and commissioning phase is important for any facility, other aspects of a facility’s process safety program are often necessary to ensure the effectiveness of the electrical classification as a means of ignition source control. For example, a strong safety culture that reinforces the meaning and intent of electrical classification may be necessary to ensure that, during operation, the hazards within an area remain consistent with its classification.

An overview of hazardous area electrical classification will be presented using a detailed case study. The presentation will include a case study demonstrating how a combustible dust explosion at a manufacturing facility could have been mitigated had a strong process safety program been in place. It will be shown how the facility relied heavily on the design-case electrical classification/zone process for the facility, and how this reliance failed to alert them to the hazards that ultimately led to a combustible dust explosion at the facility.

5:20 PM **Lessons Learned During the Hydraulic Testing of Firewater Systems** (TueC2e)

Nicolas Guzman (Baker Risk Engineering and Risk Consultants)

Firewater system hydraulic testing can pinpoint crucial flaws in a facility's firefighting capabilities, and can direct facility personnel toward best practices. What are some of the common failures found in firewater systems? What are some of the consequences of an improperly managed system?

Renewable Energy

Tuesday, February 28, 2017 (Illinois C, **TueC3**)

Chair: *Diane Graziano* (Argonne National Laboratory)

Co-Chair: *Shweta Singh* (Purdue University)

4:00 PM **Evaluate Performance of a Phase Change Composite (PCC) Material as an Energy Storage Medium for Cold Thermal Energy Storage (TES) Applications** (TueC3a)

Ahmed Aljehani (University of Illinois at Chicago), Siddique Khateeb, Said Al-Hallaj (AllCell Technologies)

The work in this project evaluates the use of a phase change composite (PCC) material consisting of (n-tetradecane and expanded graphite) as a potential's storage medium for cold Thermal Energy Storage (TES) system. The proposed PCC based TES system will be integrated with a conventional air conditioning (AC) system. The overall integrated system will work as a smart grid demand-side management solution to reduce the electricity consumed for comfort cooling applications during peak hours. The use of this PCC material is novel in cooling applications because of its unique material characteristics as compared to ice or chilled water that are predominantly the only choice of materials in TES systems for cooling applications.

The proposed PCC-TES system was evaluated from engineering perspective through multiple evaluation stages. The first stage involved the preliminary performance evaluation of the concept of integrating a PCC-TES into an air conditioning system using ASPEN PLUS ® software (Chemical Process Optimization software). The second stage involved the actual experimental testing of a 3.5 kWh PCC-TES prototype unit. The third stage involved material characterization of potential phase change materials (PCM) for cold TES applications.

During the first stage which involved the preliminary concept evaluation, a heat transfer analytical model was developed to simulate the phase change material behavior and characteristics. The heat transfer model was written as a FORTRAN code within the calculation block of ASPEN PLUS®. The air conditioning's refrigeration cycle was simulated in ASPEN PLUS® software using the in-built components library. The ASPEN PLUS® software was able to simulate the PCC-TES system integrated with AC unit and predict phase transition characteristics of the PCC material and Ice. During the second stage, a 3.5 kilowatt-hour (kWh) PCC-TES system was built and tested in laboratory using a chiller system. Ethylene glycol was used as the heat transfer fluid to charge and discharge the PCC-TES system at various flow-rates. The experimental results demonstrated very high efficiency greater than 95% during discharge cycle. During the third stage, various PCM candidates were tested and evaluated to select the best material in terms of latent heat, melting-solidification parameters, evaporation rate, availability and cost.

4:20 PM **Operation of Grid Scale Energy Storage Systems: Comparison of Multi-Stage Stochastic Programming and EMPC** (TueC3b)

Oluwasanmi Adeodu, Donald J Chmielewski (Illinois Tech)

In order to increase the penetration of renewables on the electric grid, large-scale energy storage systems have been proposed as a means of mitigating the effects of the intermittency of renewable power supply. For such networks augmented with uncertain renewable power supply, stochastic programming is a natural choice of grid operating policy. However, the time-coupling constraints introduced by the addition of storage specifically requires a computationally intensive multi-stage stochastic programming (MSP) approach to fully realize the economic benefits of energy storage. In this work, we develop the application of MSP to govern economic dispatch operations on electric networks with energy storage. Then, it is shown that a closed-loop implementation of economic model predictive control (EMPC), a radical simplification of MSP, provides an economic performance comparable to that of MSP at a fraction of the computational burden. In addition to providing a reduction in computational cost, the similarity in performance of these two operating policies serves as a basis to adopt an array of tractable EMPC- based design methods for the optimal sizing and placement of storage units.

4:40 PM **Stochastic Optimization of Energy Storage Systems** (TueC3c)

Ranjeet Kumar, Victor M. Zavala (University of Wisconsin-Madison)

We propose a stochastic programming model to study flexibility and economic opportunities provided by batteries in frequency regulation and energy markets. We formulate a two-stage stochastic program to capture uncertainty in market prices and loads. We solve the two-stage stochastic programming formulation in a receding horizon scheme, which enables us to update the formulation at every step as new information is received, and thus get an optimal policy over long decision periods. We compare performance against perfect information and deterministic settings.

5:00 PM **Stochastic Optimization to Reduce Cost of Energy for Parabolic Trough Solar Power Plant** (TueC3d)

Urmila Diwekar (Vishwamitra Research Institute), *Dev Parikh* (University of Illinois at Chicago)

The need for clean and cheap renewable energy is on the rise. Solar energy is one of the most clean and readily available technologies with almost zero carbon emissions. Optimizing the resources to produce efficient power at low costs is the need of the day. However, solar energy power plants face number of uncertainties like weather. Since the technologies are new, cost uncertainties are common. In this work, we optimize a solar thermal power plant with two different capacities using the novel Better Optimization of Nonlinear Uncertain Systems (BONUS) algorithm. We use the System Advisory Model (SAM) system from NREL to model performance and economics of the power plant. Since this is a black box model, optimization and optimization under uncertainty becomes difficult. Unlike the deterministic optimization problem, in stochastic programming (or stochastic optimization), one has to consider the probabilistic functional of the objective function and constraints. The generalized treatment of such problems is to use computationally intensive probabilistic or stochastic models instead of the deterministic model, inside the optimization loop. BONUS can circumvent the problems associated with black box models, computational intensity of sampling, and perturbation derivative costs. Instead of the stochastic modeling loop BONUS uses a statistical reweighting approach to obtain the probabilistic information. It has been shown that BONUS reduces computational intensity by 98 to 99% for large scale problems like this problem of optimization of solar thermal power plant. It has been found that the solution of expected value cost minimization for the two different capacity solar plants is robust in the face of uncertainties.

5:20 PM **Clean Energy & Sustainable Water Treatment** (TueC3e)
Suresh Jambunathan (Veolia)

A Utility Grid (UG) links common water treatment technologies (membrane filtration, thermal distillation) and uses clean energy to sustainably treat water. Providing Utility Grid services to municipal, agricultural and industrial communities is increasingly profitable, because of macroeconomic factors including climate change induced water stress, plentiful natural gas and increasingly inexpensive renewable energy (wind, solar etc…).

This presentation frames starts an increasingly common scenario - water scarcity in dry geographies, then discusses how renewable electricity supplemented by a clean burning natural gas fueled Combined Heat & Power (CHP) system can inexpensively treat surface & sub-surface waters and deliver treated water for potable, industrial and agricultural use.

This presentation outlines specific project development milestones, including risks & mitigants. A key take-away is that reducing, reusing and recycling primary resources avoids a false choice between our conscience and our wallets.

Job Search Essentials

Tuesday, February 28, 2017 (Illinois B, **TueC4**)
Chair: *Akshar Patel* (Illinois Tech)
4:00 PM Job Searching Essentials: Utilizing Technology to Strengthen Your Job Search (***Laptops Recommended***) (TueC4a)
Akshar Patel (Illinois Tech)

Advances in technology have directly impacted the modern job search. Paper resumes are no longer the way to get your foot in the door. In The 2-Hour Job Search, author Steve Dalton, writes about utilizing technology to navigate the ever changing job market to find the right job faster. By utilizing Dalton's LAMP list method, job seekers can quickly see which companies to connect with and start building connections to grow their network of advocates. Illinois Institute of Technology Career Services has adopted Dalton's method and students have directly benefited from the methods in "The 2-Hour Job Search". Laptops are recommended for this session.

AIChE Midwest Regional Conference
Presentation Abstracts
Wednesday, March 1, 2017

<u>Biomedical Engineering I</u>
Wednesday, March 1, 2017 (Cardinal Room, **WedA1**)
Chair: *Jesper Madsen* (University of Chicago)
Co-Chair: *Daniel Young* (Illinois Tech)

9:45 AM **Molecular Modeling as a Screening Tool to Separate Enantiomers of Chiral Compounds Using Polysaccharide-based Chiral Stationary Phases for Orphan Drugs** (WedA1a)
Binwu Zhao, Priyanka Sharma (Orochem Technologies Inc.), *Xiaoyu Wang*, Sohail Murad (Illinois Tech)

The pharmacological activity of chiral substances in living systems differs since the human body is a highly chiral environment. Enantioselective differences exist in the pharmacokinetics and pharmacodynamics of the various pharmaceutical drugs sold as racemic mixtures. Purification of these racemic mixtures to create enantiopure drugs has become an intense priority for large pharmaceutical companies due to the findings that some enantiomeric forms of certain drugs are harmful to the human body. The design of chromatographic purification systems for the production of single enantiomer drugs is challenging and expensive for pharmaceutical companies. This is owed to the current 'guess-and-check' method where method development chemists must screen a large number of combinations of chiral stationary phases, mobile phases, pH, and temperatures to achieve acceptable separation and purification of racemic mixtures. To aid in the currently slow speed of chiral technology advancement, Orochem Technologies along with a molecular simulation team at the Illinois Institute of Technology (IIT) propose development of a predictive molecular model which can guide experimentation and aid its own research scientists as well as those at other drug companies to create solutions to the demanding separation problems. Our first phase of work includes modeling of Orochem's CSP-1A chiral stationary phase, which we have validated in molecular dynamics simulations. The configurational behavior of the CSP-1A in various solvents in our simulation agrees with experimental observations. We have also developed protocols for generating parameters for both CSPs and chiral molecules utilizing Gaussian and RESP charge fitting. In our study, we have modeled the adsorption of flavanone enantiomers to CSP-1A in various solvent environments and shown agreement with experiments performed on chiral HPLC experiments. We are working to optimize the force field parameters currently to further enhance the effect of various solvents with changing polarity. The successful development of our predictive model will have a substantial impact on the drug development industry. Our proposed molecular model will accelerate drug discovery in pharmaceutical companies and allow for unique drug formulations to be available in the market to consumers that are relying on them for treatment and to extend their lives.

10:05 AM **Absolute EPR Oxygen Imaging for the Assessment of Oxygen Pressure and Local Oxygen Consumption Rate in Tissue Grafts** (WedA1b)
Mrignayani Kotecha (University of Illinois at Chicago), *Boris Epel, Howard Halpern* (University of Chicago)

In this presentation, we will show the utility of electron paramagnetic resonance oxygen imaging (EPROI) technique for the assessment of tissue oxygenation in porous scaffolds and engineered tissues. EPROI is a magnetic resonance spin lattice relaxation-based imaging technique with absolute oxygen resolution of 1-3 torr at low pO2 and spatial resolution of 1mm. It has been used extensively to map animal tumor hypoxia, to evaluate tumor drug efficiency, and recently, to enhance radiation therapy. However, it's potential in assessing tissue oxygenation of tissue grafts in vitro and in vivo has not been recognized yet. We will discuss the principles of oxygen image acquisition using EPRI and show early results that EPROI can differentiate porous poly-lactic-co-glycolic acid (PLGA) scaffolds with different porosity and can provide local oxygen consumption rate of stem cells seeded in osteogenic tissue grafts made from collagen/chitosan hydrogels. These early data show the usefulness of EPROI for the assessment of tissue oxygenation in engineered grafts. The knowledge of three-dimensional oxygen map potentially can be used for enhancing graft design, assessing cell viability and controlling the outcome of cell differentiation.

10:25 AM **Tunable Gradient Hydrogel for Vascularization** (WedA1c)
Yusheng He, Georgia Papavasiliou (Illinois Tech)

Neovascularization is highly dependent on gradients of soluble (chemotactic) and immobilized (haptotactic) extracellular matrix signals as well as gradients of physical structure and mechanical properties (durotactic). The development of polymerization strategies that allow for controlled spatial and temporal gradients of these signals in 3D biomaterials holds great promise for rapid and stable vascularization of engineered tissues. We have developed a photopolymerization technique (ascending-frontal-photopolymerization (AFP)) to generate combined as well as individual gradients of chemotactic, haptotactic and durotactic signals in synthetic hydrogel scaffolds. AFP was used to create MMP-sensitive poly(ethylene) glycol (PEG) hydrogels with individual gradients of1) the immobilized cell adhesive RGD peptide (350±240-865±295M) and with uniform elastic modulus (1174±80Pa), 2) elastic modulus (528±94-1587±77Pa) and with uniform RGD concentration (1400±51M) and 3) fluorescently labeled hydrogel nanoparticle carriers (fluorescent intensity range 7.1±1.9-06±0.4a.u) that promote sustained release of proangiogenic factors. A 3D neovascularization in vitro assay was used to investigate the effect of the RGD gradient on vascular sprout invasion. Preliminary data indicate that the invasion area in RGD gradient scaffolds increases 4.2-4.9-fold over 7-days, but is not significantly different as compared to control scaffolds with uniform RGD content. Current efforts are focused on quantifying in vitro response to durotactic and chemotactic cues as well as to variations in gradient magnitude and slope.

10:45 AM **Probiotic Escherichia Coli Outcompetes Pathogens During Biofilm Formation** (WedA1d)
Kuili Fang, Seok Hoon Hong (Illinois Tech)

Most bacteria live as sessile communities by forming biofilms in aquatic environments by the secretion of extracellular polymeric substances. Numerous chronic bacterial infections are involved in biofilm state and it is difficult to treat them by antibiotics. Compared to the planktonic counterparts, cells inside the biofilms become highly resistant to antimicrobial agents, via entering the non-metabolizing state, regulating stress-responsive mechanisms, and producing extracellular matrix. Hence, it is required to develop novel effective ways to control deleterious biofilms. Escherichia coli strain Nissle 1917 (EcN) is a probiotic bacterium that has been used as a medicine for the treatment of intestinal tract diseases. Recent studies have proved that EcN has antagonistic effects on enterohemorrhagic E. coli (EHEC) adherence, growth, and biofilm formation, and could be used as an effective treatment for EHEC-related infectious diseases. In this study, we investigated the ability of EcN to outcompete with the biofilm formation of pathogenic bacteria such as EHEC, Enterococcus faecalis, Pseudomonas aeruginosa, and Serratia marcescens. When dual-species biofilms are formed, EcN reduced EHEC biofilm formation up to 100-fold compared to EHEC single biofilm formation, E. faecalis 10-fold, and P. aeruginosa PA14 10-fold. EcN was dominant in the dual biofilms by occupying up to 90% of the total biofilm population. To see whether the small compounds secreted from EcN affect EHEC biofilm formation, we grew EHEC biofilms under EcN supernatant prepared from overnight EcN culture in the M9G medium followed by filtration. EcN supernatant decreased EHEC biofilms 100-fold which is similar to the result of the EcN-EHEC dual biofilms. As a control, commensal E. coli BW25113 did not reduce the biofilm formation of pathogenic bacteria. These results imply that probiotic E. coli inhibits the biofilm formation of pathogenic bacteria, and provides insights that probiotics can be applied as an effective treatment for the biofilm-related infectious diseases.

11:05 AM **Development of Novel Metabolite-responsive Transcriptional Factors via High-throughput, Combinatorial Protein Fusion** (WedA1e)
Peter Y. Su, Joshua N. Leonard, Keith E.J. Tyo, Andrew K.D. Younger (Northwestern University)

Metabolic engineering has benefitted enormously from expressing heterologous pathways and optimizing specific enzyme expression levels. However, truly dynamic feedback control remains one area still under development that could greatly improve product titers and process efficiency, especially in helping to mitigate buildup of toxic pathway intermediates. Additionally, high-throughput screening strategies for strains over- or under-expressing a particular metabolite remain inadequate. Although there is enormous diversity in proteins that bind certain metabolites, transforming these metabolite-binding proteins into biosensors that regulate gene expression in a metabolite-dependent fashion is not trivial.

To address this challenge, we developed a high-throughput method for generating and screening candidate biosensors, using an approach in which a DNA-binding domain is randomly inserted into a metabolite-binding protein. We recently demonstrated that such an approach can be used to generate biosensor proteins capable of regulating gene expression upon binding of their target ligand, using maltose binding protein as a model metabolite-binding protein and performing domain insertion using a specific approach that leverages extensive prior knowledge of this protein. In this project, we have extended this strategy to use random domain insertion to investigate all possible fusion points. Our approach takes advantage of an unbiased in vitro transposon insertion reaction to examine all possible insertions of the small DNA-binding domain into the larger metabolite-binding protein and uses FACS to sort for functional biosensor proteins. The primary goal and advantage of this approach is that it rapidly and efficiently evaluates all possible metabolite-responsive transcription factors stemming from a parent protein/enzyme with a particular DNA-binding domain. We developed and evaluated this method by creating a library of insertions of a DNA-binding domain into maltose binding protein, characterized the insertion landscape of the library by next generation sequencing, and ultimately discovered several new functional biosensors. Our results therefore validate a readily generalizable method that may potentially be applied towards converting a wide range of ligand-binding proteins into novel biosensors for applications in metabolic engineering and synthetic biology.

Refining I

Wednesday, March 1, 2017 (White Oak **WedA2**)
Chair: *Sravan Pappu* (Johnson Matthey)
Co-Chair: *Juan Salazar* (UOP//Honeywell)

9:45 AM **BP Whiting Refinery Modernization Project** (WedA2a)
John Bartels (BP)

TBA

10:05 AM **Sulfur Unit Equipment Problems and Low Silicon Carbon Steel Corrosion** (WedA2b)
Jerry Wilks (CITGO Petroleum Inc.)

Sulfur Units are actually one of the most important aspects of a refinery, but sulfur units don't get a lot of credit because they don't produce a product that is marketed to make money. The values associated with sulfur units are only realized when the unit or units are down, and the refinery has to be cut back because the remaining amine and sour water systems can't handle what the refinery usually produces. This situation makes the reliability of sulfur units important to refinery operations, but spending money on sulfur units doesn't get the appropriate level of importance. Therefore engineers and others working on sulfur units have to be very smart to keep their units operating at minimal cost. This presentation will review several sulfur unit equipment problems and solutions to those problems. Also, many of us have heard about the problems Chevron has had with low silicon carbon steel in a crude unit. The problems Chevron had weren't new because information had been previously published on the enhanced corrosion that occurs with low silicon carbon steel. The low silicon carbon steels can corrode at a rate that is fifteen times higher than that of normal silicon carbon steels when exposed to high temperatures and reactive sulfur compounds. Therefore this phenomenon occurs in sulfur units too so failures of low silicon carbon steels will be reviewed in this presentation.

10:25 AM **Coking Mechanism in Refinery Fractionator Wash Beds** (WedA2c)
Lowell Pless (Johnson Matthey Process Technologies), *Gregory A Cantley, James F Johnson* (Marathon Petroleum Corporation)

This presentation will discuss a novel theory of the coking mechanism in a refinery fractionator wash bed.

The wash bed of a refinery fractionator is prone to coking/fouling due to the low liquid rates along with high vapor rates and high temperatures. Generally, the wetting rate at the top of the wash bed is minimized to prevent high-value product loss, but lower wetting rates lead directly to coke formation in the bed. So the refinery works to balance the economics of product recovery versus unscheduled downtime to replace a coked bed. Marathon has used Tracerco ThruVision™ technology to help manage the wash bed life while maximizing product recovery during the normal turnaround cycle. The ThruVision™ technology provides a detailed density map at a specific vertical elevation that can pinpoint specific areas of liquid maldistribution or solids build-up.

During a turnaround cycle, several towers have experienced heater trips that have led to step changes in the wash bed density seen by the ThruVision™ technology and ΔP. A review of this data from several refinery fractionators has guided the creation of a new theory on how the coke is formed in a refinery fractionator wash bed.

10:45 AM **Impeller Performance Characteristics: Flow, Shear and Efficiency** (WedA2d)

Richard K. Grenville, Jason J. Giacomelli (Philadelphia Mixing Solutions Ltd.)

Impellers in agitated vessels are often described in terms such as high flow, high efficiency, high shear etc. These terms are qualitative and are not helpful when carrying out an agitator design / sizing calculation. The impellers are essentially pumps, machines that move the fluid inside the vessel, and their performance characteristics can be defined in the same way as a pump; in terms of the power input, the flow and head generated and the efficiency. Impellers are also required to generate shear, either to disperse a second liquid or gas phase in order to generate surface area for mass transfer or to promote coagulation / flocculation of fine particles suspended in the liquid phase.

The region of highest shear in a stirred tank is found in the trailing vortex at the tip of the impeller blades. The properties of the vortex must be taken into account in order to correctly calculate a local shear rate. In this presentation a method for quantifying the flow and shear characteristics of impellers will be presented demonstrating how this method may be applied to shear driven processes. The calculation method will be verified by comparing with results from droplet break-up and flocculation experiments.

The main conclusion of this work is that the Rushton turbine, traditionally considered "high shear", actually generates larger droplets and floccs than a Hydrofoil, traditionally considered to be "low shear" at the same power input. This is important when selecting the appropriate impellers for processes where high or low-shear mixing are requirements.

11:05 AM **Flow Dynamics in High-velocity and -solids Flux Circulating Fluidized Bed Risers of FCC Catalyst Particles** (WedA2e)

Allan Issangya, Ray Cocco, Reddy SB Karri (Particulate Solid Research, Inc)

The presentation discusses radial solids flux profiles in three 0.3-m-diameter CFB risers operated at superficial gas velocities reaching of between 12 and 16 m/s and solids fluxes of 100 to 800 kg/s.m2. These operating conditions are close to those typically found in commercial fluid catalytic cracking (FCC) units.

Sustainability

Wednesday, March 1, 2017 (Illinois C, **WedA3**)

Chair: *Rae Mindock* (Rae Mindock Consulting)

Co-Chair: *Elena Savona* (Elevate Energy)

9:45 AM **Mixing of Red Sea and Dead Sea Waters** (WedA3a)

Abdelaziz Lafi Khlaifat, Mufeed Batarseh, Khalid Nawayseh, Jamal Amira, Emad Talafeha (Abu Dhabi Polytechnic)

The water level in the Dead Sea is shrinking at a rate of more than one meter per year, and its surface area has shrunk by more than 35% in the last 30 years. This is largely due to the diversion of over 90% of the water of the Jordan River and evaporation caused by industrial activities to generate fertilizers and other chemical products. In the early 1960s, the river moved 1.5 billion cubic meter of water every year from the Sea of Galilee to the Dead Sea. Dams, canals, and pumping stations built by Israel, Jordan and Syria now divert water for crops and drinking, and have reduced the flow to less than 100 million cubic meter a year (MCM/yr) (mainly brackish water and sewage). The decline of the Dead Sea level is creating major environmental problems: the creation of sink holes that endanger structures, plantations and roads; receding sea shores and the creation of mud plains; and other effects on the environment and the flora and fauna of the region.

The only way to save the Dead Sea and eliminate the impact of the level decline is to provide it with a continuous flow of water coming from the Red Sea. The Red Sea–Dead Sea Conduit, sometimes called the Two Seas Canal, is a proposed conduit (pipes and brine canal) which would run from the Red Sea to the Dead Sea (about 180 km). It will provide potable water to Jordan, Israel and the Palestinian territories, bring sea water to stabilize the Dead Sea water level and generate electricity to support the energy needs of the project.

This paper focuses on a critical theme: Mixing of Red Sea-Dead Sea waters and its impact on inshore-offshore transport, industry and subsequent ecological consequences. The designed pilot project was constructed on the southern shores of the Dead Sea using well-controlled mixed water ponds to investigate the interaction between Red Sea and Dead Sea waters through: addressing major concern raised regarding gypsum crystallization, and its physical, chemical, environmental and operational consequences; quantification of halite precipitation after diluting Dead Sea water with the Red Sea water; determination of the effect of gypsum and halite precipitation on the increase in the salinity of the brine; investigation of other mineral phases and trace metals precipitation; the variations in chemical and physical properties of Red-Dead Sea mixture throughout the year; and the effect of mixing of Red Sea and Dead Sea waters on biological diversity.

10:05 AM **A review of the book on "Energy: Sources, Utilization, Legislation, Sustainability, Illinois as Model State" G.A. Mansoori, N. Enayati and L.B. Agyarko** (WedA3b)

L. Barnie Agyarko, G.Ali Mansoori (University of Illinois at Chicago)

In this talk, we report on the book that focuses on energy sources, utilizations, legislations and sustainability, as it relates to a state, a province, or a country, or a community within a state. This book presents various kinds of energy sources, ways to convert energy for end use, better use of energy towards conservation and energy- and environmental-sustainability. As a very proper model-state we chose the State of Illinois which has the largest overall fossil energy reserves, including the largest strippable bituminous coal reserves; the largest user of nuclear energy in USA and has also been investing in all kinds of renewable energies including wind energy, solar energy, biofuels, geothermal energy, and various energy storage options. In the authors' opinion, State of Illinois is a pioneer in legislations for proper development and use of all kinds of energy. Motivation to do this project was to educate the public (including students, energy engineers and planers, as well as state- and country-wide policy makers) about all aspects of energy.

In this book, all the possible energy sources including coal, natural gas, petroleum, nuclear, solar, wind, biofuels and geothermal energy are presented, as well as energy storage options. Also presented are various ways of dealing with carbon dioxide, which is produced from fossil fuels combustion, including its collection, transportation, storage and sequestration. The energy storage systems presented in this book will facilitate reliable and full integration of renewable power to the grid.

10:25 AM **Squeezing More Out of C&I Energy Audit Programs: How to Increase Conversion Rates towards Savings** (WedA3c)

Chris Philbrick (CB&I)

Objective: Provide detailed background information and data about the current energy audit programs for commercial & industrial (C&I) customers; identify typical conversion rates, and outline the factors that impact likelihood of customers moving forward with efficiency measures identified from energy assessments.

Results/Achievements/Concepts: Most energy efficiency programs offer some form of energy audit support. This may be in the form of a rebate for all or some portion of the cost of the audit. There is often the question, "how much energy savings is achieved as a result of the audit?" because energy savings are only achieved if the recommendations in the audit are implemented.

Our research has identified over 300 audit programs offered to commercial and industrial customers. Audits range in size, scope, and type; from On-line, Off-line, and On-site energy assessments. The studies identify energy recommendations that vary from low cost measures to capital projects. The recommendations often lead a customer to additional utility rebate programs like lighting and motor rebates. Programs may be broken into different phases that are intended to lead to energy savings, such as the assessment phase and implementation phase, etc. The paper draws upon experience as audit program administrators, implementers and feedback from customers to deliver guidelines for the improvement of converting energy assessments into energy savings.

Program results from the Smart Energy Design Assistance Center (Illinois Department of Commerce and Economic Opportunity), Focus on Energy (Public Service Commission of Wisconsin), and the Duke Energy Non-Residential Assessment Program (NRAP) will be used to provide real-world data towards support of this topic.

Worthiness: This is an opportunity to have an in-depth conversation about the true value of energy audits for C&I customers and the utility programs that are available. Energy audits are a great first step to increasing a facility's energy efficiency. By understanding the specific conditions that affect a businesses' energy usage, C&I customers can learn about the variety of measures that can be implemented to lower their energy bills, improve efficiency processes, and increase the comfort within a facility (or multiple facilities). This will also be an opportunity to discuss what the challenges are that are facing customers when it comes to implementing energy efficiency measures/recommendations, therefore providing a benefit to the utility, the implementer, as well as the customer.

10:45 AM **Emerging Technology for Buildings – Predictive Optimization** (WedA3d)
Dan Docel (BuildingIQ Inc.)

Building owners and managers face a conundrum - how to cut operating costs while going green, without lowering occupant comfort and worker productivity. Furthermore, budgets are tight, staff isn't expanding, and employees are more demanding. Finally, money isn't growing on trees to enable capital expenditures to rip and replace building systems. So, where do we go from here and what's a building manager to do? An answer can be found in novel software approaches that rely on a mixture of cutting edge predictive analytics and old fashioned facility expertise. Instead of replacing or adding equipment, companies can instead add intelligence to their existing environment in three steps: analyze the data at hand, meaning the building physics itself, the BMS' actual capabilities, and chief external factors like the hour-to-hour weather; predict energy needs of the building optimal performance; and then control and measure the BMS and impact on the building's energy use.

This session will highlight how a thermal model of a building or campus can be created on a daily basis based on a weather forecast, utility tariffs and occupancy. Furthermore, it will illustrate how the model will change throughout the day based on existing weather versus forecasted weather. The session will demonstrate how the model actually controls the building based on all of the parameters analyzed. This is truly advanced machine to machine communication taking human guess work out of the mix. The underlying technology took over 50 man years of advanced scientist time to develop. The models were first generated in Australia where the price of energy is 4-5 times higher than here. Both the Australian National Laboratory (CSIRO) and the U.S. National Laboratory (Argonne) collaborated to develop Predictive Energy Optimization (PEO).

The results of thermal models can be profound. At an operating level, it means optimal energy efficiency, lowered operating costs, reduced labor costs and increased occupant comfort. At a higher level, such a high level of control governed by analysis and software directly enhances a building's ability to respond to non-organic, external inputs, like a demand response signal. And finally, the three-step methodology is by nature transparent in that the model, prediction, forecasting, and control are all measured and tracked. Attendees of this session will hear how other buildings round the world have implemented optimization, how roadblocks to implementation can be overcome, and how such a system can impact overall occupant comfort and positive outcomes.

11:05 AM **TBA** (WedA3e)
TBA (TBA)

Biomedical Engineering II

Wednesday, March 1, 2017 (Cardinal Room, **WedB1**)
Chair: *Atul Khare* (Pfanstiehl)
Co-Chair: *Ying Liu* (University of Illinois at Chicago)

2:00 PM **Use of Acoustic Microstreaming for Drastic Sensing Enhancement** (WedB1a)
Dmitry Gritsenko, Andrea De Vellis, Yang Lin, Jie Xu (University of Illinois at Chicago)

There is a high demand for ultrafast biosensors for industrial and public health applications. However, the performance of existing sensors is often limited by the slow mass transport process in traditional pressure-driven microfluidic devices. We show for the first time, that acoustic microbubbles trapped in prefabricated cavities in a micro-chamber are capable of enhancing fluid sample mixing that results in faster delivery of target species to the sensor surface. We demonstrate a drastic reduction of sensor response time (up to 21.3 fold) for surface-based nanosenors in presence of resonantly actuated microbubbles. The obtained results are valid in a wide pH (4-10) range and agree well with previous studies.

2:20 PM **Engineering Red Blood Cell-Based Biosensors for Physiological Monitoring** (WedB1b)
Taylor Dolberg, Kelly Schwarz, Joshua Leonard (Northwestern University)

Cell-based therapies have a wide range of applications ranging from cancer immunotherapy to regenerative medicine. A promising emerging frontier of this field is the development of engineered red blood cells (eRBCs) for therapeutic and diagnostic applications. RBCs are an attractive platform for diagnostics because they have exceptionally long circulation times (around 120 days – far longer than synthetic vehicles), lack DNA (and thus are safe), and can be loaded with drugs, proteins, or other cargo. Recent technological advances have enabled the large-scale production of RBCs from precursor cells, which may potentially be harnessed to generate off-the shelf eRBC-based products to meet medical needs, including both diagnostic and therapeutic applications.

The specific goal of this project is to generate eRBC-based technologies enabling non-invasive monitoring for pathogen exposure (e.g., in the context of first responders) and for other "actionable" analytes (e.g., markers of inflammation post-surgery). Towards this goal, we are developing eRBC biosensors that generate a fluorescent output upon detection of the analyte of interest, and this output may be monitored non-invasively using established technologies for fluorescent imaging of the retina. These biosensors would enable the detection of actionable analytes thus benefitting exposed personnel by accelerating the initiation of treatment (perhaps before obvious symptoms present) and reducing of further exposure risks when possible.

As a first step to enable RBCs to act as sensors, we designed and evaluated a novel biosensor strategy that is suitable for achieving biosensing in eRBCs, which lack DNA and thus require a readout other than gene expression. Towards this end, we engineered a novel cell-surface receptor protein in which ligand binding induces receptor dimerization, which then facilitates reconstitution of an intracellular split fluorescent protein. Importantly, our strategy involves modification of RBC-resident proteins, since retention of membrane proteins during RBC maturation is a tightly regulated and an incompletely understood process. We comparatively evaluated a range of biosensor architectures that implement the proposed mechanism, enabling us to identify biosensor designs and design features that successfully conferred significant ligand-induced generation of fluorescent output. We also evaluated and implemented strategies for improving biosensor performance, including minimization of background fluorescence and enhancing fold-induction upon exposure to ligand. This crucial proof-of-principle demonstration establishes a foundation for developing eRBC biosensors that could ultimately address an unmet need for non-invasive monitoring of physiological signals for a range of diagnostic applications.

2:40 PM **Cancer Cell Hyperactivity and Membrane Dipolarity Monitoring via Raman Mapping of Interfaced Graphene: Towards Non-Invasive Cancer Diagnostics** (WedB1c)

Bijentimala Keisham, Arron Cole, Phong Nguyen, Ankit Mehta, Vikas Berry (University of Illinois at Chicago)

Ultra-sensitive detection, mapping and monitoring of the activity of cancer cells is critical for treatment evaluation and patient care. Here, we demonstrate that a cancer cell's glycolysis-induced hyperactivity and enhanced electronegative membrane (from sialic acid) can sensitively modify the second-order overtone of in-plane phonon vibration energies (2D) of interfaced graphene via a hole-doping mechanism. By leveraging ultrathin graphene's high quantum capacitance and responsive phononics, we sensitively differentiated the activity of interfaced Glioblastoma Multiforme (GBM) cells, a malignant brain tumor, from that of human astrocytes at a single-cell resolution. GBM cell's high surface electronegativity (potential 310 mV approximately) and hyperacidic-release induces hole-doping in graphene with a 3-fold higher 2D vibration energy shift of approximately 6±0.5 cm-1 than astrocytes. From molecular dipole induced quantum coupling, we estimate that the sialic acid density on the cell membrane increases from one molecule per 17 nm2 to one molecule per 7 nm2 (approximately). Further, graphene phononic response also identified enhanced acidity of cancer cell's growth medium. Graphene's phonon-sensitive platform to determine interfaced cell's activity/chemistry will potentially open avenues for studying activity of other cancer cell types, including metastatic tumors and characterizing different grades of their malignancy.

3:00 PM **Estimation of Oxygen Consumption for People with Type 1 Diabetes Based on Exercise Pattern** (WedB1d)

Sediqeh Samadi, Nicole Frantz, Kamuran Turksoy, Ali Cinar (Illinois Tech)

A new model with two submodels is proposed for estimation of oxygen consumption in aerobic treadmill and stationary bike exercises, with various patterns of exercise intensities.

The first submodel uses the speed and inclination of the treadmill or the speed and resistance of the bike as the inputs to estimate heart rate during the exercise and recovery time. It is an extension of a nonlinear model [1] with the speed of treadmill as its only input. However, changes in grade (inclination) of treadmill affects the heart rate remarkably. The second submodel predicts oxygen consumption based on the heart rate estimated by the first submodel.

Data to build and evaluate the submodels are obtained from exercise studies conducted for young adults with T1D. Subjects wore Zephyr BioHarness and performed two episodes of 30-minute training with treadmill and bike at different intensities. Oxygen consumption and heart rate are measured during cardiopulmonary treadmill stress test. The data set of eleven subjects are used.

Mean average error of estimated oxygen consumption for speed, inclination or resistance as model inputs is 0.32 L/min for training and 0.51 L/min for testing data. Aerobic energy expenditure is linearly proportional with oxygen consumption. The model gives good estimates of energy expenditure based on time and intensity of aerob.

[1] TM Cheng, AV Savkin, BG Celler, SW Su, L Wang, Nonlinear modeling and control of human heart rate response during exercise with various work load intensities, IEEE Trans. Biomed. Eng., 55: 2499–2508, 2008.

3:20 PM **Controlled Delivery of a Pro-Angiogenic Peptide from Hydrogel Nanoparticles for Therapeutic Neovascularization** (WedB1e)

Daniel Young, Georga Papavasiliou (Illinois Tech)

Therapeutic neovascularization involving proangiogenic growth factor delivery has shown promise for restoring perfusion in ischemic tissues; however, the clinical efficacy of growth factors has been limited by their associated immunogenicity and structural instability in vivo. A promising alternative uses growth factor-mimetic peptide sequences to interact with receptors for regulating neovascularization while providing high biological specificity, enhanced structural stability, and ease in synthesis. Stable, functional neovascularization requires controlled and sustained delivery of angiogenic factors. We have designed synthetic hydrogel nanoparticles of poly(ethylene) glycol using inverse phase miniemulsion polymerization with tunable crosslink density to enable adjustments in release of the physically entrapped vascular endothelial growth factor-mimetic peptide, QK, over 60 days. We altered QK release by synthesizing nanoparticles with low (LXD) and high (HXD) crosslink density (0.754 and 0.810 mmol/cm^3) via adjustments in crosslinker concentration. LXD and HXD nanoparticles resulted in particle diameters of 225.0 and 259.1, zeta potentials of 4.07 and -8.29 mV, and swelling ratios of 11.7 and 10.0, respectively. The bioactivity of QK released from nanoparticles of varying crosslink densities at 8 hrs and 14 days (tested at 1E-6 M) was evaluated using a matrigel tubulogenesis assay. All groups containing QK showed increases over the basal control. QK released from LXD nanoparticles at 8 hr and from HXD nanoparticles at 14 days resulted in significant differences in normalized mean tubule length (40% and 31% increase over control, $p < 0.05$). Current efforts are investigating the delivery of QK-loaded nanoparticles on stimulating ischemic tissue repair in vivo.

Refining II

Wednesday, March 1, 2017 (White Oak, **WedB2**)

Chair: *Hadjira Iddir* (UOP/Honeywell)

Co-Chair: *Allan Issangya* (PSRI)

2:00 PM **Production of Renewable Diesel and Jet Fuels** (WedB2a)

Henrik Rasmussen (Haldor Topsoe Inc.)

The production of Renewable fuels is mandated by the RFS2 regulation and Haldor Topsoe has developed a process technology and specialized catalysts to make renewable fuels based on a variety of feedstocks. Our process is commercially proven in more than a dozen plants and the paper will highlight the reaction pathways for making renewable fuels and the specialized catalysts that is selective for the different reaction pathways and the associated benefits with each pathways. The presentation will also show commercial data from industrial units and how to address pressure drop mitigation and corrosion issues with these new feedstocks as well as dewaxing to meet the cold flow properties. The presentation will demonstrate that we have the capability to make drop in renewable fuels which meet the ASTM D-975 specification.

2:20 PM **Redefining Operability in Hydrogen Plants** (WedB2b)

Abigail Sup, Susan Simpson (Johnson Matthey)

Traditionally, hydrogen plant operators have managed performance reliability of steam methane reformers (SMRs) through visual furnace inspections, tube wall temperature monitoring, or responsiveness of process temperatures and conditions outside of the SMR. These methods are labor and time intensive which could result in monitoring that actually takes longer than the observed effect on performance or even mechanical failure within the SMR. Through the use of CatTrackers, a process side thermometry used within the SMR tube, hydrogen plant operators are able to achieve a step change in responsiveness to SMR operability. Real process experiences will be discussed about early process condition detection. These experiences will show this real-time responsiveness as well as highlight situations that lead to more severe performance problems. In addition, transients will be examined to demonstrate that when traditional operating parameters are not available or quality is less reliable, CatTrackers can provide an operator with the information needed to safely react to these changes which could have resulted in the expense of extended downtime or failure in the past.

2:40 PM **Integrating Economic MPC and RTO** (WedB2c)

Douglas A. Allan, James B. Rawlings (University of Wisconsin Madison)

Traditionally, model predictive control (MPC) has used on setpoint tracking objectives. These setpoints are determined by steady state economic process optimization techniques, such as real-time optimization (RTO). MPC and RTO typically use different process models--- MPC usually uses linear black-box models identified empirically, whereas RTO uses first-principles grey box models with some empirically identified parameters. Because these models are different, the setpoints determined by RTO are usually not steady states for MPC, and therefore there exists an MPC steady-state target problem that finds a steady state for MPC nearby to the steady state calculated by RTO. This target problem can contain both tracking and economic criteria. This framework is used successfully in industry.

Recently, a type of MPC that use an economic objective, called economic MPC (EMPC), has been proposed to enhance process profitability. However, some processes are more profitable when they are operated in a periodic cycle rather than at steady state, and as a result EMPC can destabilize these processes. Sometimes, however, the economic advantage to operate cyclically rather than at steady state is an artifact of the of the simplified process model used by MPC. Furthermore, whether or not there exists a true economic advantage to cyclic operations, industrial processes are often not designed to be operated in this way, and attempts to operate them cyclically can contribute to equipment fatigue and can be a safety hazard. In order to see EMPC adopted by industry, these issues must be resolved.

We propose to integrate EMPC and RTO to create a control system that is stabilizing and offers enhanced economic performance. EMPC is known to be stabilizing if a linear system model is used with a convex cost function. Each time RTO is run, we find a convex quadratic approximation to its objective function in a neighborhood of its proposed setpoint. This approximate economic cost is then used as the objective function of linear EMPC, and the resulting closed loop system is stabilizing. We illustrate this approach with a simple example, in which we compare the closed loop economic performance of our method with the traditional structure of RTO, steady-state target finding, and tracking MPC.

3:00 PM **Natural Gas Sweetening and Dehydration Process Simulation and Optimization using MEG Solution** (WedB2d)

Firas Alnili (Curtin University of Technology)

Natural gas is the most important and popular fossil fuel in the current time and also in the future. Although natural gas is mostly considered as a "clean" fuel as compared to other fossil fuels, the natural gas found in reservoirs deposit is not necessarily "clean" and free of impurities. Natural gas consists primarily of methane as the prevailing element but it also contains considerable amounts of light and heavier hydrocarbons as well as contaminating compounds of CO2, N2, H2S and other impurities. These impurities are undesirable compounds and cause several technical problems such as corrosion and environment pollution. However, many natural gas stream in different areas Contains huge quantities of H2S and CO2. Therefore, this study aims to simulate the gas sweetening process by using Aspen HYSYS V.7.3 program. Moreover, the simulation work is adopted MEG (Mono-Ethylene Glycol) gas sweetening process by using MEG solution and it achieved high acid gases removal and dehydration, for instance, H2S concentration in sweet gas stream was about > 2.5 ppm and (0.03 mol%) of CO2 at (1000 m3/h) MEG circulation rate. In addition, the simulation work is also achieved process optimization by using several MEG concentrations (70%, 75% and 80%) and temperatures (20 °C, 25 °C and 30 °C). It also investigated the effect of MEG concentrations and inlet temperature on the regeneration reboiler temperature and duty. Moreover, the optimization work found that the use of (MEG 80% w/w at 20 °C) may consider the most recommended conditions.

3:20 PM **Remaining Life Assessments of Refinery Furnace Tubes Using Omega Simulations** (WedB2e)

Jerry Wilks (CITGO Petroleum Inc)

Process simulations are used frequently in refining to determine the optimum operating parameters for a wide range of processes. The development of Omega technology by the oil industry in the 1990's led to the development of a new type of simulation that made it possible to assess the effects of past service on high temperature equipment and to predict future equipment performance. Furnace tubes are a type of high temperature equipment that is well suited to Omega simulation analyses. Furnace tubes fail due to the combination of creep and corrosion processes. Creep is a process that involves diffusion, crystal deformation, crystal boundary slipping, and dislocation motion – processes that eventually results in equipment failure. These degradation processes can be simulated by Omega software, and the simulation results predict the remaining life of the furnace tubes under the existing process conditions or when exposed to new process conditions. This type of simulation is more complex than typical process simulations because past equipment history is an essential part of the simulation. Omega simulations deal with years of past operating data and typically predict performance years into the future.

Carbon Capture

Wednesday, March 1, 2017 (Illinois C, **WedB3**)

Chair: *Naresh Susarla* (Argonne National Laboratory)

Co-Chair *Nishith R. Patel* (University of Wisconsin)

2:00 PM **CO2 Capture in a Multistage CFB with Sorbent Regeneration using Waste Heat** (WedB3a)

Dimitri Gidaspow (Illinois Tech), *Sutthichai Boonprasop, Benjapon Chalermsinsuwan, Pornpote Piumsomboon* (Chulalongkorn University)

State of the art of CO2 capture technologies for existing fossil energy power plants are limited to amine absorbers (G. T.Rochelle. 2009). The regeneration of these solvents consumes 15 to 30% of the energy of the power plant due to the use of steam that is not used to produce power. The proposed concept uses the heat of reaction and waste flue gas heat for regeneration. The high decomposition pressure of the sorbent allows regeneration at a low temperature.

This proposed concept of CO_2 capture uses dry sodium carbonate developed for use in bubbling fluidized beds at RTI (Coleman, et al, 2009).We have shown that the circulating fluidized beds (CFB) are superior to bubbling beds because in such beds the temperature rise due to the heat of reaction is only a few degrees due to the circulation of the sorbents (Chalermsinsuwan, et al 2010, Kongkitisupchai and Gidaspow, 2013).

Unfortunately the high decomposition pressure of the sorbent requires the use of several stages with cooling between the stages. We have shown that we need at least 3 stages for a 90% CO_2 removal. Our design was obtained using a multiphase computational fluid dynamics code following the equilibrium curve for the decomposition of the sodium bicarbonate. The rate of sorption was limited by diffusion into clusters that form in the risers. Hence accurate rates of sorption were not needed for our design.

2:20 PM **Integrated Process of CO_2 Capture and Conversion to Alkyl Carbonate** (WedB3b)

C. B. Panchal, John C. Prindle, Rachel Strutz, Richard Doctor (E3Tec Service, LLC)

There are very limited uses of captured CO_2 other than for enhanced oil recovery (EOR) which currently has in excess of 126 projects globally; some as high as a 2 Mtonne/yr capacity. The Global Carbon Capture and Sequestration (CCS) Insititute provides a list of current and future storage sites and also highlights the challenges and costs of coordinating the development of a CO_2 transportation infrastructure. Few major industrial CO_2 generation sources (e.g. refineries, petrochemical production, ammonia/urea manufacturing facilities, fossil power generation plants etc.) are located close to these storage sites. Hence, substantial CO_2 transportation costs would be incurred after capture. Additionally, legal title to non-EOR geological storage portends costly and protracted litigation and has led to the abandonment of several CO_2 sequestration projects. As a result, different technologies for conversion of captured CO_2 to value-added products are being actively pursued. E3Tec is pursuing an integrated process of CO_2 capture and conversion to alkyl carbonate, specifically dimethyl carbonate (DMC). This integrated process focuses on distributed CO_2 sources with limited access to CO_2 sequestration sites. The conventional amine process as well as emerging CO_2 capture processes are evaluated for integration with the CO_2-based DMC process. The heat integrated reactive distillation (HIRD) process equipped with side reactors offers an energy-efficient process with low overall Carbon Footprint. The E3Tec project is supported by DOE SBIR program and Alberta's Climate Change and Emissions Management Corporation (CCEMC), now called Emissions Reduction Alberta (ERA).

2:40 PM **3D-Printed Monoliths for CO_2 Removal from Enclosed Environments** (WedB3c)

Harshul Thakkar (Missouri University of Science and Technology)

Structured adsorbents, especially in the form of monolithic contactors, offer an excellent gas−solid contacting strategy for the development of practical and scalable CO_2 capture technologies. In this study, the fabrication of three dimensional (3D)-printed zeolite and amino-silica monoliths with novel structures and their use in CO_2 removal from air and flue gas respectively are reported. The physical and structural properties of these printed monoliths are evaluated and compared with their powder counterparts. Our results indicate that 3D-printed monoliths with higher loadings of pristine powder as high as 90 wt % exhibit adsorption uptake that is comparable to that of powder sorbents. The dynamic CO_2/N_2 breakthrough experiments show relatively fast dynamics for monolithic structures. In addition, the printed monoliths show reasonably good mechanical stability that can eventually prevent attrition and dusting issues commonly encountered in traditional pellets and beads packing systems. The 3D printing technique offers an alternative, cost-effective, and facile approach to fabricate structured adsorbents with tunable structural, chemical, and mechanical properties for use in gas separation processes.

3:00 PM **Efficiency of Artificial Photosynthetic Devices for Integrated Carbon Capture and Reduction** (WedB3d)

Aditya Prajapati, Meenesh R. Singh (University of Illinois at Chicago)

The anthropogenic contribution of CO_2 is ~15 Gt per year, which has led to the rise in CO_2 concentration at the rate of ~1.8 ppm per year in the atmosphere severely affecting the earth's climate. As this rate will continue to increase in the future, there is an urgent need to develop efficient technologies for the abatement of CO_2 and to sustainably produce carbon-neutral fuels. Here we evaluate thermodynamic and achievable limits for the efficiency of an artificial photosynthetic system composed of an integrated CO_2 capture and photo/electrochemical reduction processes to produce carbon-neutral fuels. The carbon capture by an ideal process and other practical techniques such as Monoethanolamine (MEA) scrubbing, membrane separation, adsorption, and electrodialysis have been analyzed. The overall thermodynamic and achievable efficiencies of artificial photosynthetic systems have been calculated using Shockley-Queisser limits of multi-junction light absorbers and load curves of carbon capture and reduction processes. The calculated efficiencies for ideal CO_2 capture and reduction processes were in the range of 20-27% for a single junction, 34-40% for a double junction, and 24-34% for a triple junction light absorber for different products of CO_2 reduction reactions.

3:20 PM **Simultaneous Adsorption of SOx, NOx, and CO_2 on Bimetallic MOFs** (WedB3e)

Amit Hajari, Harshul Thakkar, Shane Lawson (Missouri University of Science and Technology)

Recent developments in the field of flue gas processing have resulted in focus being given to find highly selective materials for combined CO_2, SOx, and NOx capture. In this scenario, metal organic frameworks (MOFs) are a promising notion. In this study, an innovative approach has adopted to capture CO_2 along with SOx and NOx simultaneously by incorporating two different metals into the MOF framework for effective interactions with three different acid gases present in the flue gas. A series of bimetallic MOFs with varied metals weight ratios were synthesized and their adsorptive performance for simultaneous removal of SO_2, NO, and CO_2 was systematically investigated by conducting equilibrium and dynamic uptake measurements. In addition, their performance was compared with their monometallic MOFs counterparts. Moreover, the bimetallic MOFs were characterized by various techniques including FTIR, XRD, SEM and ICP, before and after exposure to acidic gases in order to identify any change in their chemical and structural properties. The results indicate that the synthesized bimetallic MOF adsorbents exhibit superior simultaneous gas uptake compared to conventional monometallic MOF materials.

<u>Biomedical Engineering III</u>

Wednesday, March 1, 2017 (Cardinal Room, **WedC1**)

Chair: *Mrignayani Kotecha* (University of Illinois at Chicago)

Co-Chair: *Claire Y. Liu* (Purdue University)

4:00 PM **Polyphosphate Loaded Poly(ethylene) Glycol Hydrogel Nanoparticles Targeting Bacterial Collagenase Suppression for Intestinal Healing** (WedC1a)

Dylan Nichols, Fouad Teymour, Georgia Papavasiliou (Illinois Tech),
Melissa Arron, Olga Zaborina, John Alverdy (University of Chicago)
Successful repair and return of function following intestinal injury as a result of disease or surgical manipulation can be enhanced or disrupted by the intestinal microbiota. Common treatment involves antibiotic administration which has been shown to disrupt intestinal microbial composition leading to further healing impairment. We have shown that under phosphate deprived conditions, pathogenic intestinal microbes produce high levels of collagenase, a key phenotype involved in impaired intestinal healing. Strategies that allow for targeted delivery of phosphates to the intestinal epithelium while allowing commensal bacteria to proliferate normally have a significant advantage in addressing this problem. We have developed a novel drug delivery approach involving the use of hydrogel nanoparticles that allow for prolonged release of phosphates to be delivered to the intestinal epithelium. Polyphosphate (PPi), was encapsulated in poly(ethylene) glycol diacrylate hydrogel nanoparticles (NP-PPi) formed using inverse miniemulsion polymerization. NP-PPi have an average particle diameter, zeta potential and swelling ratio of 181.7 nm ± 52.2 nm, -17.92 mV ± 1.05 mV and 2.8 ± 0.08, respectively, and allow for sustained release of PPi over three days. Free PPi reduces collagenase levels in gram-negative pathogens (P. aeruginosa and S. marcescens) while maintaining bacterial survival. Preliminary in vitro studies illustrate that NP-PPi suppressed collagenase levels of S. marcescens. Current studies are being performed to test the effectiveness of NP-PPi in suppressing collagenase levels across gram-positive and gram-negative pathogens.

4:20 PM **Designing a Microfluidic Platform for High-Throughput Screening of Pharmaceutical Polymorphs** (WedC1b)

Paria Coliaie, Meenesh R.Singh (University of Illinois at Chicago)
Pharmaceutical molecules can crystallize in various crystalline structures called polymorphs, which can have significantly different physicochemical properties such as bio-availability, chemical stability and mechanical strength. Identification of meta-stable and stable polymorphs are crucial to the pharmaceutical industry due to regulatory constraints. The current technique used in pharmaceutical industry is the 96-well plate, which can screen large number of solvents and operating conditions within a week. The primary issue with this method is pertaining to the use of stagnant condition in the 96-well, which allows multiple crystals to grow due to varying local environment. As a consequence of uncontrolled screening of crystals in the 96-well plate, several set-backs are often encountered during scale-up of crystallizers. Here we propose a novel high-throughput microfluidic crystallizer, whose hydrodynamic conditions can be controlled to grow and analyze single crystals of pharmaceutical polymorphs. We have systematically designed a microfluidic device consisting of a thermalizer, a mixer and a diffuser section to simulate the environment of a large-scale crystallizer in the microchannels. In this talk, I will present an optimal design of such microfluidic device and discuss the procedures for high-throughput screening.

4:40 PM **Mechanistic Study on Co-agglomeration of Active Pharmaceutical Ingredients and Excipients** (WedC1c)

Kanjakha Pal, Ramon Peña, Zoltan K. Nagy (Purdue University),
Christopher L. Burcham, Daniel J. Jarmer (Eli Lilly and Company)
Spherical Agglomeration is a novel Process Intensification method that has captured the interest of the pharmaceutical industry. The major goal of spherical agglomeration is to eliminate processes (milling, granulation) in the process flow of pharmaceutical manufacturing and thereby bring down the cost of making the drug product. The major problems with traditional spherical agglomeration was that excipients were not being incorporated inside the agglomerates because of incompatibility of surface wetting properties between the various components in a formulation. Co-agglomeration of Pharmaceutical APIs was carried out using Emulsion Solvent Diffusion (ESD) Process which enables uniform distribution of the API and the excipients inside the agglomerates. In this paper the mechanistic aspects of co-agglomeration of the APIs and the excipients were investigated by using various Process Analytical Technology (PAT) tools. The effect of various process conditions on the co-agglomeration process was also investigated and it was found that PAT tools like Focused Beam Reflectance Measurement (FBRM) can provide critical insights into the fundamental mechanisms going on in the Emulsion Solvent Diffusion process. It was also found that PAT tools can help us gain real time information on the effect of various process parameters on the size distribution of the agglomerates and thus can be used in open loop control of Agglomerate Size Distribution.

5:00 PM **Multiscale Models for Insulin Secretion and Autoimmunity in Islets of Langerhans** (WedC1d)

Mustafa Cagdas Ozturk, Qian Xu, Ali Cinar (Illinois Tech)
Accurate modeling of Islets of Langerhans plays a critical role in the understanding of the pathogenesis and progression of Type 1 Diabetes mellitus. For this reason, several models have been developed, which represent either the cellular level functions, or the metabolic level regulation of blood glucose. On the other hand, such models are only able to represent the behavior at their respective scales [1]. For example, metabolic models do not capture the oscillatory patterns of insulin secretion from the Beta cells, whereas cellular scale models do not interpret the changes in plasma concentrations of insulin and glucose. Yet, the gap between the two scales needs to be closed in order to obtain a holistic view of diabetes. Multiscale modeling provides a remedy to this situation, and allows the observation of the consequences of cellular scale interactions at the metabolic scale, and vice versa.

In this work, we present a multiscale model of insulin secretion, which consists of a compartmental metabolic simulator and an agent-based model for reproducing the islet function. The modular structure of the multiscale model enables the use of any metabolic simulator, depending on the goals of the simulations. For the preliminary results we present, the minimal model [2] was used for plasma glucose and insulin calculations.

The agent-based model represents ß-cells, which secrete insulin in a discrete fashion to mimic the exocytosis of insulin granules [3]. This naturally leads to the biphasic secretion of insulin from the cells and the calculation of the overall insulin secretion rate, which is then used in the metabolic simulator for plasma concentration calculations.

Additionally, another agent-based model is introduced, which focuses on the interactions between immune system components (such as CD8+ T Cells), and the islet components (such as the Beta cells, the islet basement membrane). It is expected that the coupling of a model of the autoimmune destruction of Beta cells in the pancreas with a multiscale model of insulin secretion will open the way to early diagnosis of Type 1 Diabetes and facilitate the development of clinical intervention strategies.

Both agent-based models are implemented on a high performance computing (HPC) framework, which opens up the possibility to simulate the whole islet mass of a human pancreas (~1 million islets). Furthermore, the versatility of agent-based modeling allows the representation of in vitro and microfluidic applications. Lastly, the models can be calibrated according to experimental or clinical data through parameter estimation methods.

[1] R. N. Bergman, “Minimal model: Perspective from 2005,” Horm. Res., vol. 64, no. SUPPL. 3, pp. 8–15, 2005.
[2] R. N. Bergman, L. S. Phillips, and C. Cobelli, “Physiologic evaluation of factors controlling glucose tolerance in man: measurement of insulin sensitivity and beta-cell glucose sensitivity from the response to

intravenous glucose.," J. Clin. Invest., vol. 68, no. 6, pp. 1456–1467, Dec. 1981.
[3] P. Rorsman and E. Renstrom, "Insulin granule dynamics in pancreatic beta cells," Diabetologia, vol. 46, no. 8, pp. 1029–1045, Aug. 2003.

5:20 PM **Nip the Bud: Aggregation Hierarchy of Influenza M2 Scission Proteins in Membrane Necks** (WedC1e)
Jesper J. Madsen, John M. A. Grime, Gregory A. Voth (University of Chicago)

Viral release of influenza is believed to occur independently of the usual cellular machinery of endosomal sorting complexes required for transport (ESCRT); instead, scission of the extruding bud is facilitated by the M2 protein (Rossman et al. Cell 141, pp. 902-913, 2010). The shape of the M2 transmembrane domain is distinctly conical and the assumed mechanism by which scission proceeds is that M2 aggregates in the budding neck to cause constriction that eventually pinches off the enveloped virus.

To investigate this hypothesis, we have constructed a minimal physical model consisting of a coarse-grained lipid bilayer membrane (Brannigan et al. Phys. Rev. E 72, 011915, 2005) whose geometry is shaped to a budding neck by an attractive guiding sphere. In this way, we can model the fascinating phenomenon of budding in a generic yet accurate theoretical framework on the relevant in vivo length scale. We present numerical results for enveloped virus release and predict M2 aggregate topologies in various representative stages of the budding process.

Process Control and Optimization

Wednesday, March 1, 2017 (White Oak, **WedC2**)
Chair: *Yankai Cao* (University of Wisconsin Madison)
Co-Chair: *Ha Dinh* (UOP/Honeywell)

4:00 PM **Model Predictive Control for Tracking Zones with Discrete Actuators** (WedC2a)
Nishith R. Patel, James B. Rawlings (University of Wisconsin Madison)

Model predictive control (MPC) is an advanced control technology with thousands of applications in the chemical and petroleum industries (Qin & Badgwell, 2003). MPC uses a dynamic system model to make predictions of the output variables as a function of the actions taken by the controller (Rawlings & Mayne, 2009). In the conventional MPC procedure, an online optimization problem is solved over a horizon to drive process variables to desired setpoints. In several key industrial applications, however, the control objective is to keep process variables within a zone or target set. Such examples include level control in a buffer tank between upstream and downstream process units as well as temperature control in commercial buildings.

For such cases, modifications to the traditional MPC paradigm are required. Some industrial applications use soft constraints implemented with software such as Aspen DMCplus, but the theoretical conditions under which the closed-loop system is stable are not well understood. Lyapunov-based economic MPC keeps the state within a region defined by a sublevel set of the Lyapunov function (Ellis et al., 2016). However, since the region is a sublevel set, it cannot be an arbitrary design choice by the user. MPC for tracking zone regions has also been proposed (Ferramosca et al., 2010). When inside the zone though, it may be desirable to achieve secondary economic objectives. Furthermore, actuators may be discrete (e.g., valves may be on-off). The problem formulation should ideally address these issues.

In this talk, we develop the MPC theory for tracking zones with discrete actuators, we propose an implementable framework for satisfying secondary economic objectives, and we demonstrate the effectiveness of this formulation on two example problems. First, the MPC formulation for tracking zones is presented. In zone tracking, the tracking stage cost is zero if the state is in the target set and positive otherwise. An example of a function that satisfies this property is the distance function from a point to a set. Under the stated assumptions, the target set is shown to be asymptotically stable for the closed-loop system even in the presence of discrete actuators. Since the solution of the optimization problem is often nonunique when tracking zones, a general framework is proposed to achieve secondary control objectives such as minimizing economic costs, input value, or input movement. After solving the zone tracking problem, a second optimization problem can be solved to determine a unique input trajectory from the stabilizing set that optimizes secondary control objectives. Next, the proposed formulation is applied to two example problems. The first problem considered is a buffer tank between upstream and downstream process units. The objective is to minimize the effect of the upstream flow disturbance on downstream units by allowing the height of material in the tank to vary. The input available to the controller is an on-off valve at the tank outlet. While the height is allowed to vary, it should be kept within bounds to prevent emptying or overflowing. Through simulations, we demonstrate that the proposed MPC formulation accomplishes these goals. The second problem considered is indoor air temperature control. The temperature in commercial buildings is not required to be at a setpoint. The air temperature should be maintained between upper and lower bounds to keep the occupants in the building comfortable. When the temperature is outside of these bounds, the controller should take action to drive the temperature to the comfort region. When the temperature is inside the bounds, the controller should minimize the number of times the heating, ventilation, and air conditioning (HVAC) system is turned on or off. The performance of the proposed zone tracking MPC is compared to that of a hysteresis controller.

Qin, S. J., & Badgwell, T. A. (2003). A survey of industrial model predictive control technology. Control Engineering Practice, 11 (7), 733-764.
Rawlings, J. B., & Mayne, D. Q. (2009). Model Predictive Control: Theory and Design. Madison, WI: Nob Hill Publishing.
Ellis, M., Liu, J., & Christofides, P. D. (2016). Economic Model Predictive Control: Theory, Formulations and Chemical Process Applications. London, England: Springer.
Ferramosca, A., Limon, D., González, A. H., Odloak, D., & Camacho, E. F. (2010). MPC for tracking zone regions. Journal of Process Control, 20(4), 506-516.

4:20 PM **Multi-level Supervision and System Modification for Artificial Pancreas** (WedC2b)
Jianyuan Feng, Ali Cinar (Illinois Tech)

Artificial pancreas (AP) systems are implemented as a treatment of people with type 1 diabetes (T1D) to regulate blood glucose concentration (BGC). A typical AP system including 3 components, a continuous glucose monitoring (CGM) sensor measuring subcutaneous glucose concentration (to infer BGC) at high sampling rates, a controller calculating insulin infusion rate based on the CGM signal, and a pump delivering the insulin amount calculated by the controller to the patient. The performance of the AP system depends on the corporation of these three components.

Many AP systems are using model predictive controller which rely on models, either first principles or data-driven, to predict BGC. Using the BGC predictions, the controller calculates the insulin infusion rate to keep the BGC values in safe range. The performance of model-based control systems depends on the accuracy of the models and may be affected when large dynamic changes in the human body or changes in equipment performance occur and move the operating conditions away from those used in developing the models and designing the control system. Sensor errors such as signal bias and missing signal will cause misleading or stop the calculation of insulin infusion rate. And the performance of the controller may be varying at each sampling step, each period (meal, exercise, sleep) and even each day.

In order to supervise the performance of the AP system and retune the controller to enhance the safety and improve the accuracy of insulin infusion rate calculation, a multi-level supervision and system modification (ML-S&SM) module was developed. This system supervises the performance of AP system in 3 levels: sample level, period level, and 24-hour level. In sample level, an online controller performance assessment sub-module will generate controller performance indexes to evaluate different aspects of AP system and modify the controller conservatively. And a sensor error detection and signal reconciliation module will detect sensor error and reconcile the CGM sensor signal at each sample. In period level, the controller is estimated with more information to track the controller performance within a certain time period and reconcile the controller in a more aggressive manner. And in a 24-hour level, the daily BGC distribution will be further analyzed to determine the adjustable range of controller parameters used for sample level and period level. Thirty subjects in the UVa/Padova metabolic simulator are used in simulations to evaluate the performance of the ML-S&SM module. The results indicate that the AP system with ML-S&SM module has a safer range of glucose concentration distribution and more reasonable insulin infusion rate suggestions than an AP system without the ML-S&FR module.

4:40 PM **The Extended and Unscented Kalman Filtering Methods for Real-Time Estimation of Plasma Insulin Concentration in an Artificial Pancreas System** (WedC2c)
Iman Hajizadeh, Kamuran Turksoy, Ali Cinar (Illinois Tech), *Eda Cengiz* (Yale University)

Artificial pancreas (AP) systems use continuous glucose measurements (CGM) to calculate optimum amount of insulin to be infused with an insulin pump. Real-time estimations for plasma insulin concentration (PIC) rather than generalized curve based insulin-on-board (IOB) estimates can be beneficial for improving the performance of AP control algorithms to calculate more realistic insulin infusion rates and prevent hypoglycemia that would be caused by overdosing of insulin. Our objective is to fulfill a real-time estimation of PIC from CGM data by using two different mathematical models.

Two different glucose-insulin compartmental models, Hovorka's model and extended Bergman's minimal model, which were developed to describe glucose-insulin dynamic in different parts of the human body, have been incorporated into a continuous-discrete extended Kalman filter (CD-EKF) and an unscented Kalman filter (UKF), respectively, to provide an estimate of the plasma insulin concentration. Furthermore, because of variability in system dynamics, uncertain parameters have been considered as new states in Hovorka's model and Bergman's minimal model to be estimated by CD-EKF and UKF, correspondingly. Thirteen datasets from nine different subjects with type 1 diabetes are used. Two euglycemic clamps were performed on separate mornings with (seven datasets) and without (six datasets) an insulin infusion site warming device. Subjects had one CGM sensor and blood was collected to measure plasma insulin levels for up to 5 hr. On both days, a bolus of 0.2 U/kg aspart insulin was infused at the beginning of each experiment and the basal infusion was suspended, and glucose levels were maintained between 90 and 100 mg/dl by infusion of variable rate of dextrose. In addition, partial least squares models based on each patient's demographic information such as body weight, height, BMI and total daily insulin dose are developed for the initial guess of the time-varying unknown model parameters used in the nonlinear CD-EKF and UKF estimators.

According to the CD-EKF estimator, the average root mean square errors are found to be 12.36 and 11.56 mU/L for the clamps with and without IP, respectively. The average mean absolute relative error with respect to the measured samples are 0.14 for the two clamps. The average Pearson's R coefficient are 0.95 and 0.91 for the clamps with and without IP, correspondingly. For UKF estimator, estimated plasma insulin concentrations are found to be linearly correlated with the measured insulin samples (R= 0.94 and 0.89 for the clamps with and without IP, respectively). The average root mean square errors are found to be 12.69 and 12.09 mU/L for the clamps with and without IP, respectively. The average mean absolute relative error with respect to the measured samples are 0.12 and 0.10 for the clamps with and without IP, correspondingly.

The proposed methods are able to estimate the plasma insulin concentration in real time by using only CGM measurements. These methods will may be beneficial for an AP system in terms of real time estimation of insulin concentration for preventing excessive insulin infusions if plasma insulin levels are already elevated.

5:00 PM **Synthesizing optimal nuclear waste blends using Multi-agent optimization framework** (WedC2d)
Berhane Gebreslassie, Urmila M. Diwekar (Vishwamitra Research Institute)

Optimal blending of nuclear wastes produced from nuclear reactor at Hanford site in Southern Washington is solved in this work. Vitrification of the nuclear wastes to form glass is a process that will be used for the disposal of high-level waste. The amount of glass form produced can be reduced by optimal blending of the nuclear wastes. The optimal configuration of nuclear waste tanks that minimize the volume of glass form can be obtained by combinatorial optimization algorithms. However, this problem results in a combinatorial explosion as the number of nuclear waste tank increase. Moreover, the feasibility thermodynamic property constraints make this problem highly non-convex where to get the global optimal solution become nontrivial.

Multi-agent optimization method is a nature inspired framework that supports cooperative search of an optimal solution of an optimization problem by a group of algorithmic agents connected through an environment with certain predefined information sharing protocol. In this work, we use a heterogeneous multi-agent optimization (HTMAO) framework to solve the nuclear blending problem. The optimal waste blending problem is formulated as a mixed integer nonlinear programming (MINLP) in which the total frit needed for the vitrfication process is minimized subject to the feasibility of thermodynamic properties and process model constraints. The model simultaneously determines the optimal decisions that include the configuration of the nuclear waste tanks that form each waste blend and the amount of frit needed for the vitrification of each waste blend. In the HTMAO framework we use efficient ant colony optimization algorithms, efficient simulated annealing; efficient genetic algorithm and NLP solver based on derivative methods (SQP) are considered as algorithmic agents.

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5:20 PM **On the Alleviation of Inventory Creep in Process Scheduling** (WedC2e)

Yazeed Aleissa, Donald J Chmielewski (Illinois Tech)

In the work of Lima et al., [1], the notion of inventory creep within a process scheduling context was introduced. In short, the inventory creep phenomenon is a gradual reduction of material inventory over time. To alleviate this myopic behavior, the authors of [1] advocate the use of larger prediction horizons, but quickly run into computational tractability issues. Recently, similar inventory creep phenomena have been observed in the context of Economic MPC, [2, 3, 4]. In [2] and [3], inventory creep was virtually eliminated by the use of a surrogate MPC objective function. This quadratic objective function was constructed to be inverse optimal with respect to an appropriately defined Economic Linear Optimal Control (ELOC) policy [5]. In [3], the original economic objective function is retained, but is appended by an ELOC derived final cost term. This final cost is an approximation of the original objective function (from the end of the prediction horizon to infinity) resulted in an approximate infinite-horizon EMPC policy.

In the current effort, the approximate infinite-horizon EMPC policy is applied to a simplified version of the long-term scheduling problem found in [1]. This example is distinct from those of [2-4] in that many of the decision variables of the scheduling problem are restricted to integer values. This fact has two implications. First, these integer restrictions will significantly increase the computational complexity of the original scheduling version of the EMPC problem, and create a much greater need for reductions in horizon size. The second issue is that ELOC is incapable of enforcing integer constraints. However, development of an ELOC policy with integer constraint relaxed, leads to a final cost term that sufficiently approximates the economic cost from the end of the horizon to infinity. The result is an approximate infinite-horizon policy that enforces integer constraints over the finite horizon, but due to the appropriately selected final cost term is able to employ much short prediction horizons (requiring much less computational effort) while observing virtually zero inventory creep.

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Environmental Compliance and Remediation

Wednesday, March 1, 2017 (Illinois C, **WedC3**)

Chair: *Amid Khodadoust* (University of Illinois at Chicago)

Co-Chair: *Jarad Champion* (Geosyntec Consultants)

4:00 PM **Optimizing Spatio-temporal Sensor Placement for Nutrient Monitoring: Algorithmic Framework** (WedC3a)

Urmila Diwekar, Kinnar Sen (Vishwamitra Research Institute)

INFEWS is a new initiative in NSF which deals with Innovations at the Nexus of the Food, Energy and Waters Systems. This project addresses the INFEWS: N/P/H2O solicitation. The food production system generates waste streams that are characterized by high concentrations of organic matter, nitrogen- and phosphorus-containing species in water. Therefore, monitoring nitrogen and phosphorous species is important for water quality requirements for agricultural as well as energy production. Currently these species are monitored via stationary monitoring stations. However nitrogen and phosphorous species move via agricultural run-off to other water systems, and requires portable sensors which can change the positions in real time. This type of dynamic sensing requires novel algorithms which decide sensor locations in real time in the face of inherent uncertainties in the fate and transport of the species. To develop such an algorithmic framework to solve the problem of sensor placement in real time is the objective of this proposal.

This paper presents the first part of the work which is the algorithmic framework for optimal spatial-temporal locations of the sensors in real time. The algorithmic framework is based on a novel algorithm called Better Optimization of Nonlinear Uncertain Systems (BONUS). We present a case study of an agent based model from social sciences for testing these framework. This model is based on behavior of cows in a field where there are grass patches. The cows move in a herd towards the greener pasture and eat grass till it finishes. The grass growth and cow movements are probabilistic. We are using four sensors for object tracking (e.g. cows) and these sensor move spatially and temporally in order to track maximum number of cows. Results show that the optimal movement of sensors allows to track maximum number of cows.

In the future, the algorithmic framework will be coupled with nutrient and fate transport models. A case study of a small watershed will be selected from literature for nutrient monitoring sensor location problem. Optimal spatial-temporal locations will be the result of this new framework for this case study.

4:20 PM **Integrated Livestock Wastewater Treatment System for Simultaneous Destruction of Bioactive Microconstituents from Biosolids and Bioenergy Recovery** (WedC3b)

Young Hwan Shin, Peng Zhang, Michael Plewa, Yuanhui Zhang (University of Illinois at Urbana - Champaign), *Lance Schideman, John Scott* (Illinois Sustainable Technology Centre)

Livestock wastewater contain bioactive microconstituents that potentially contribute to ecological or health effects. For instance, estrone (E1), 17β-estradiol (E2), and estriol (E3) can have adverse effects on the reproductive biology of vertebrates at very low concentrations (Irwin et al., 2001; Schuh et al., 2011). Antibiotic resistant bacteria that cause life threatening infections can be developed from bacteria exposed to low levels of antibiotics excreted in urine and feces (Wise et al., 1998; Sarmah et al., 2006; Berge et al., 2006; Martinez, 2009). This study investigates the effects of Mixed algal-bacterial bioreactor (MABB) and hydrothermal liquefaction (HTL) simultaneously produce biomass for bioenergy production and reduce the discharge of bioactive microconstituents. Thus, the integrated system improves the quality of water resources and increase energy security by removing organics/nutrients and producing bio crude oil/gas, respectively.

Fresh swine manure samples were collected and analysed to quantify the occurrence of natural bioactive microconstituents in the manure which were subsequently filtered with 0.45 µm membrane to generate the liquid portion of swine manure (LPAM). ELISA and GC/MS followed by Solid Phase Extraction (SPE) were used to analyse bioactive microconstituents and the concentration of E1 and E2 in LPAM were ranged from 10,602 to 11,875 ng/L and 11,753 to 22,646 ng/L.

cytotoxicity of the LPAM was investigated using a previously developed Chinese Hamster Ovary (CHO) cell assay (Hsie AW, 1975; Wagner et al., 1998), and the extracted LPAM organics had a cytotoxicity index of 2.38, which is slightly less than secondary municipal wastewater effluent, 2.64 (Pham et al., 2013). A fluctuation test was developed to measure antibiotic resistance in bacterial populations exposed to antibiotics in manure. E. coli 15597 was exposed to florfenicol (FF) at lethal (17 µg/mL) concentration that provides a selective advantage to individual bacterium that were acclimated to under non-lethal FF selection (2 µg/mL), and this study confirmed that exposure to FF at a non-lethal concentration increased survival during an antibiotic challenge.

MABB with adsorbents was operated to extract bioactive microconstituents and other organics from the LPAM under various operating conditions (organic loading: 35.3 to 470 mg sCOD/L/d; light intensity 350 µmol photons/m2/s; temperature: 18 to 25 ˚C; Hydraulic retention time: 4 days; Solid retention time: 30 days), and biomass was harvested to use as a biofuel feedstock with maximum productivity of 819 mg/L/d. After adding granular activated carbon (GAC) into MABB, % removal of sCOD, TN, TP, and NH3-N were increased up to 96, 72, 31, 98 %, and % removal of E1/E2 were escalated from 82.0/92.5% to 90.4/98.4%, respectively.

HTL and CHG with 10 different conditions (Temperature: 200 to 550 °C; Time: 30/60 min; Catalyst: Ruthenium on alumina, Raney-Nickel, NaOH) were performed to determine the optimal conditions for renewable energy production and to study the effects on the fate of bioactive bioactive microconstituents. E1and E2 in the spiked biomass was removed up to 94.6 and 99.8% with HTL run at 350 °C/60 min which was the most optimal condition to produce bioenergy. GC/MS were used to analyse FF concentrations and it's break down products before and after hydrothermal liquefaction. 99.96% of FF in liquid swine manure was degraded during the HTL conversion process at 300°C/30 min and 4-MSB was the predominant breakdown product observed (59%), while only small amounts of 4-MSAP (1.4%) and MPS (1.5%) were observed in the post-HTL wastewater (PHWW). The cytotoxicity of the PHWW under three conditions (sample I, II, and III: 250˚C/60min, 300˚C/60min, and 350˚C/60min) was investigated CHO cell assay. Mean cytotoxicity index (CTI) values of sample I, II, and III were 3710.2, 2380.8, and 5373.3, respectively, which tells us that the descending cytotoxicity potency was Sample III > Sample I > Sample II and toxicity in PHWW is proportional to the temperature of HTL (250° and 300°C < 350°C).

Effects of CHG on the fate of hormones were investigated with 10 different operating conditions (350, 400, 450˚C; 60min; Ru, Ra-Ni, catalyst). E2 in the spiked biomass was removed up to 99.9% with CHG run at 400˚C/60 min with Ru catalyst which is the condition of the highest gas yield. Furthermore, average % removal of E2 in the Post-CHG wastewater (PCWW) showed Ru (92.8%) > Ni (84.9%) > NiO (68.3%) and this results tells us that Ru was the most effective catalyst to break down E2 in the CHG process.

In conclusion, the research showed that daily production of bioactive microconstituents in swine manure can be quantified (E1: 27 ± 10.2; E2: 52.8 ± 0.9; E3: 9.2 ± 1.2 µg/d/hd), and the combination of MABB and HTL/CHG can simultaneously remove bioactive microconstituents from swine manure (E2, MABB: 92.3 ± 1.5%; HTL: 99.7 ± 0.1%, CHG: 99.9 ± 0.01%) and convert them into valuable bioenergy products under optimal condition (HTL: 300 °C/60min, CHG: 400 °C/60min/Ru). This will contribute to the development of cost-effective systems to reduce water pollution and increase bioenergy production as well as opportunities for reuse of the aqueous fraction.

4:40 PM **Hierarchical Mixed-Metal Oxide Adsorbents for Formaldehyde Abatement** (WedC3c)

Anirudh Krishnamurthy (Missouri University of Science and Technology)

Formaldehyde is a notorious pollutant which is carcinogenic even at low concentrations. Most studies indicate that formaldehyde concentration levels pass the World Health Organization threshold for minimal exposure by a large amount. Adsorption using porous materials has been found to be the optimal process for formaldehyde capture at low concentrations. In this work, two different transition mixed metal oxides (TMMOs) namely, TiO2/SiO2 and ZrO2/SiO2 were prepared with varying oxide ratios using a non-templated sol-gel procedure to yield hierarchical mixed metal oxides. The chemical, physical and structural properties of hierarchical TMMOs were characterized by various techniques including XRD, N2 physisorption, SEM, and ICP-OES. The formaldehyde vapor isotherms were collected at room temperature and various vapor pressures. Moreover, the adsorption tests were carried out in a fixed-bed breakthrough setup by exposing the TMMOs adsorbents to dilute formaldehyde concentrations at room temperature. Our equilibrium and dynamic adsorption results indicated that the TMMOs materials with optimum compositions have a relatively high adsorption capacity which makes them promising candidates for room temperature formaldehyde abatement.

5:00 PM **Coal Power Plant Compliance with New USEPA Effluent Limit Guidelines Rule - Water Balance Study and Computational Model Development** (WedC3d)

Jarad L. Champion, Mike Hickey, Bruce Sass, Brianna Wallace, Allison Kreinberg, Chriso Petropoulou (Geosyntec Consultants)

The USEPA promulgated the new Effluent Limitations Guidelines (ELG) rule for coal-fired steam electric power plants in November 2015. The new USEPA ELG rule became effective in January 2016 and requires the elimination of flyash transport water discharge and bottom ash transport water discharge, as well as stringent limits on discharge from flue gas desulfurization (FGD) blowdown. Compliance under the new USEPA ELG rule is required by 2023. In order to meet the USEPA ELG rule, two coal power plants operated by a confidential client are undergoing a water balance and wastewater characterization study.

Wastewater sources considered in the study include cooling tower blowdown, bottom ash and pyrite sluices, coal pile runoff, fly ash transfer building sumps, and low volume wastewaters. These wastewater sources currently combine in an ash pond where wastewater is treated by sedimentation, flocculation, and neutralization. Excess treated wastewater that is not recirculated to the plant is discharged from a reclaim pond at each plant under a National Pollutant Discharge Elimination System (NPDES) permit to the Ohio River. The primary objective of the water balance studies is to identify wastewater sources that may be contributing to final effluent discharges of inorganic constituents that may exceed future federal effluent limits.

The water balance and waste characterization study has consisted of three parts. First, a detailed water balance diagram was developed showing the flow paths of all incoming water sources (city water, river water, rain water, etc.) and all outgoing wastewater sources (i.e., sump pumps, storm stations, process flows, and other waste streams). To accomplish this, engineering drawings of wastewater sources were reviewed, operational information was discussed with plant personnel, and a plant walk down was conducted to confirm findings.

Second, the flow rates and mass loadings for each wastewater source were measured or estimated. Some flows are episodic (weather, seasonal, or dependent on electric grid demand), and some flows have continuous output (i.e., FGD filtered backwashes, WWT, Bottom Ash, Fly Ash Slurry, etc.). The chemical composition of all incoming and outgoing flows was determined by sampling and laboratory analysis. At the client's request, four sampling events were scheduled, and during each event, all sampling and flow monitoring was performed in a single day for all locations. All four sampling events will be completed by December 8, 2016.

Third, a database of flow rates and chemical compositions was developed in conjunction with a computational water balance model. Analytical and field data were validated and uploaded into a Microsoft Access database that exported flow and concentration data to an electronic dynamic link library for data management. The geochemistry of the wastewater sources mixing in the ash ponds was modeled using a GoldSim water balance model linked to a PHREEQC geochemical equilibrium model. The model allows for computational evaluation of the benefits from treating or eliminating individual wastewater sources under different operational scenarios. The computational water balance model will be used by the client during future engineering design efforts to meet the USEPA ELG rules.

This presentation provides an overview of work involved with developing the water balance diagram, measuring and estimating flow rates and chemical compositions, and development of the computational water balance model. The results of the computational model under different operational scenarios (e.g., elimination of bottom ash, pyrites, and fly ash wastewater from the ash pond; pretreatment of high-strength wastewater streams) will be presented.

5:20 PM **Combined Flue Gas Cleanup Process for Simultaneous Removal of SOx, NOx, and CO2—A Techno-Economic Analysis** (WedC3e)
Amit Hajari, Marktus Atanga, Jeremy L. Hartvigsen (Missouri University of Science and Technology)
Flue gas cleanup often requires the removal of SOx, NOx and CO2 in separate units before emitted into the atmosphere. This step-wise treatment process incurs significant cost and energy penalty to the electricity production. A combined adsorption process based on pressure swing adsorption (PSA) by which these impurities are removed is envisioned as an efficient means of flue gas cleanup that can be applied relatively easily. In this study, the technological and economic feasibility of a combined separation process in which SOx, NOx and CO2 are simultaneously removed from flue gas streams are assessed. Capital and operating costs are estimated based on sizing the equipment items and utilities needed and the potentials for increased energy efficiency are determined in relation to the required PSA performance. The energy saving potential for the adoption of 2-bed and 4-bed PSA cycle is compared with conventional FGD, SCR and amine scrubbing units needed to clean up flue gas in a step-wise fashion. The results show that energy savings can be expected when the PSA removal efficiency is greater than 90%. In the case of a 550 MW coal-fired power plant, the proposed system will impose an energy penalty of 24% to the cost of electricity which is lower than that of current individual treatment units associated with SOx, NOx, and CO2 removal. This energy penalty corresponds to a cleanup cost of $57/ton of all impurities captured for a 2-bed, four-step PSA process with cycle time of 400 s, adsorption and desorption pressure of 10 and 1 bar, respectively and a purge flow rate of 100 mol/s. This techno-economic assessment shows that the integrated combined system can be an attractive technology compared to multi-step systems for the removal of flue gas impurities.

Reaction Engineering

Wednesday, March 1, 2017 (Illinois A, **WedC4**)
Chair: *Michael Driscoll* (Stepan)
Co-Chair: *Brian Slusar* (BP)

4:00 PM **Conveyer Transport System as a Continuous Process for the Production of Supported and Structurally Complex Catalysts** (WedC4a)
Kai-Chieh Tsao, Hong Yang (Universitiy of Illinois at Urbana-Champaign)
Although the conventional colloidal synthesis or impregnation approach can be used to generate nanocrystals, the scaled-up process for making well-defined supported nanoparticle catalysts with controlled size, shape and composition needs to be developed to meet the manufacturing requirement. In this presentation, we present a new conveyor transport system that can be used to produce continuously a family of supported and shaped Pt-based nanocatalysts in a single step process. Carbon monoxide is used as a gas to reduce the metal salt precursors and influence the surface of metal surface. I will show the morphology and composition of complex structures can be finely tailored to generate electrocatalysts for enhanced activities towards methanol oxidation and oxygen reduction reactions.

4:20 PM **Enginnering Porous Polymer Hollow Fiber Flow Reactor for Sustainable C-H Functionalization** (WedC4b)
Yingxin He, Ali Rownaghi, Fateme Rezaei (Missouri University of Science and Technology)
The immobilization of organo- and heterogeneous catalysts via covalent bonding could provide a general solution, preventing leaching out of the catalytically-active centers. To date, a relatively simple and convenient method for permanent immobilization of various types of organocatalysts and the metal nanoparticles within monolithic micro-reactor that addresses stability, reactivity, and recyclability of the produced heterogeneous materials has not been established. A proof of concept study for a new type of continuous flow reactor based on porous organocatalyst and metal nanoparticles-immobilized on Torlon composite hollow fibers were considered for sustainable C-H functionalization. These novel hollow fiber reactors consist of bifunctional groups in fiber wall which render them as bifunctional catalysts for cooperative interactions (i.e., acid-base catalysis). In this study, the effects of reactants flowrate, reaction time and temperature, electron-donating, and electron-withdrawing groups of para-substituted benzaldehyde derivatives on the catalytic activity of C-H activation and C-C formation were systematically investigated. The yield of products were found to be dependent on the cooperative interactions of acid-base pair, catalyst loading, para-substituted benzaldehyde, and the reaction conditions such as temperature and contact time. The obtained results indicate that the organocatalyst and metal nanoparticles-immobilized on Torlon composite hollow fibers provide a new platform as flow reactors for heterogeneously catalyzed reactions that may facilitate the ultimate scale-up of practical fiber catalysts for the synthesis of complex organic compounds.

4:40 PM **Computational Fluid Dynamics of Slurry Bubble Column Reactor Operating at High Pressure** (WedC4c)
Mohammed Al Saraj (Ministry of Higher Education and Scientific Research)
Modeling and experimentation of slurry bubble column reactor are conducted in the present study. A pilot scale slurry reactor was used to obtain the data. Computational fluid dynamics (CFD) was used to model the reactor and simulate the concentration profiles of catalyst (loading). High pressure was used for operation and it is introduced as a parameter in CFD modeling.

5:00 PM **Developing a Novel Hydrothermal Process for Continuous Manufacturing of Thermochromic VO2 Nanomaterials** (WedC4d)
Xiaojie (Alina) Yan, Ralph T. Muehleisen, Leah B. Guzowski, Jie Li (Argonne National Laboratory), *Sam Dull* (Northwestern University), *Yungang Sun* (Temple University)
Nanoparticles have many applications due to their outstanding characteristics. However, large-scale manufacturing of high-quality nanoparticles with controlled properties is non-trivial; Technical challenges exist especially for materials that are difficult to synthesize. It is predicted that a VO2 nano-particulate film can double solar infrared heat modulation and transmittance efficiency of visible light as

compared to those of its bulk film counterpart, making the nanomaterial quite promising as the next-generation thermochromic material for high performance smart windows. However, current manufacturing methods using an autoclave reactor have many shortcomings including low conversion efficiency, poor control of product quality and safety, and being an extremely slow process (days). Modern green chemistry/process provide fundamentals to enhance such manufacturing to enable quickly and economically market acceptable products, e.g. via continuous-flow synthesis in a small module chemical reactor.

This presentation will introduce the "smart windows" concept, followed by our development of a continuous flow hydrothermal synthesis system based on a microscale reactor. The experimental demonstration will be presented to show that for the first time, it is feasible to continuously synthesize VO2 (M) micro- and/or nanoparticles in a single step, yet in a significantly reduced period of synthesis time, by using our novel processing technology. Also, we will explain the influence that in-situ surface modification of the nucleated particles using surfactants has had on the particle carry-out with the effluent. In addition, our ongoing activities related to the material scale-up and commercialization will also be briefly discussed. Finally, we will give our perspective on applying our process to preparation of other advanced nanomaterials.

5:20 PM **Detailed Modeling of LDPE Autoclave Reactors** (WedC4e)
Alejandro Cano, Thomas Lafitte, Shashank Maindarkar (Process Systems Enterprise)
Developing new polymer grades typically presents a number of challenges – for example, determining the necessary operating conditions for producing desired polymer molecular weight distributions (MWD) in reactor systems with imperfect mixing and complex kinetics. This presentation describes how an integral modeling approach that combines the advantages of gSAFT physical property predictions, detailed kinetic modeling, and characterization of flow and mixing patterns using Computational Fluid Dynamics (CFD) captures the effect of changes in operating conditions on the shape of MWDs. This type of modeling work helps in reducing development time for new polymer grades.

<u>Local Section Dinner and Keynote</u> – Ticketed Event
Wednesday, March 1, 2017 (Illinois B)
5:45 PM **Reception**
6:30 PM **Dinner**
7:30 PM **Local Section Announcements**
Tom King (UOP/Honeywell)
7:40 PM **Keynote Introduction**
Annette Johnston (Abbott Laboratories)
7:45 PM **Adjusting to EPA Policy Changes with the new Trump Administration**
Mary Ellen Ternes (Crowe & Dunlevy)
Following President Trump's inauguration on January 20, 2017, we have seen remarkable activity. As described in the January 2017 CEP, "Adjusting to Policy Changes: Full Reversal in Washington, D.C." it remains true that "some are appalled and some are applauding, but we should all fasten our seat belts!" President Trump has wasted no time initiating the changes he promised on the campaign trail. The transition has already seen numerous Executive Orders and strategic appointments, while Congress is preparing legislative strategy to undo regulation. In this presentation, Mary Ellen Ternes, industry environmental counsel and AIChE Public Affairs and Information Committee member, will review the changes so far and what these changes may mean for AIChE members in industry, academia and government.