
7TH ANNUAL



AIChE®

MIDWEST REGIONAL CONFERENCE

March 12-13, 2015

Illinois Institute of Technology



- PROCESS SAFETY • REFINING • BIO-PROCESSING •
- ENERGY • PROFESSIONAL DEVELOPMENT •

Presented by the AIChE Chicago Section

www.aiche.org/Chicago

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 7th year. Organized by the **Chicago Local Section** with support from AIChE Technical Programming and hosted by the **Illinois Institute of Technology**, the MRC provides an opportunity for engineers and scientists in the region to learn about new technologies and network with others in the field. A particular objective of the conference is to build technical relationships between industrial practitioners and researchers in the governmental and academic spheres.

Statistics of the technical program include **4 Keynote Lectures**: *C. J. Warner* (Tesoro Corporation), *Chris Gosling* (UOP, A Honeywell Company) and *Henrik Rasmussen* (Haldor Topsoe), **4 Plenary Lectures**: *Michael Graham* (University of Wisconsin-Madison), *Heriberto Cabezas* (U.S. EPA), *Lonnie Shea* (University of Michigan) and *Peter Lodal* (Eastman Chemical). There are **23 technical sessions** featuring over **100 oral presentations**.

The Thursday evening program is combined with the AIChE Chicago Local Section Monthly meeting and begins with a **Poster Session**, followed by a buffet dinner. The dinner program includes presentation of the **Thiele Award** to Alan Zagoria (UOP, A Honeywell Company) and the **Dinner Keynote Lecture** by *June Wispelwey* (Executive Director, AIChE Global).

The conference also features a **Student Outreach Program**, where Chicago-area high school and middle school students will become acquainted with the various facets of the chemical engineering profession. The outreach program will include a special luncheon where students can interact with practicing chemical engineers.

For young professionals, a **Professional Development Track** (consisting of 5 sessions) is offered. Topics range from interview and resume skills development to YP Engineering 101, Life Skills and an Entrepreneurship Panel. The conference will conclude with an off-site **YP Networking Social** aimed at solidifying contacts made at the conference.

On behalf of the conference planning committee we welcome you to the 7th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Azita Ahmadzadeh
Conference Chair
UOP, A Honeywell Company

AIChE Midwest Regional Conference Program at a Glance

Thursday, March 12, 2015

- 7:30 AM - 10:00 AM **Continental Breakfast** (Gallery Lounge)
- 8:00 AM – 9:15 AM **Morning Keynote** (Ballroom)
- *C.J. Warner*, Executive Vice President, Tesoro Corporation
- 9:30 AM – 11:30 AM **Technical Sessions**
- *Refinery Integrity Management* (Ballroom)
- *Advances in Bioremediation of Chemical Contaminants* (Armour Dinning)
- *Advances in Pharmaceuticals* (Alumni Lounge)
- *Renewable Energy Sources and Systems* (Herman Lounge)
- *Professional Development: YP Engineering 101* (Armour Conference Room)
- 11:30 AM – 1:00 PM **Lunch with High School Outreach Participants** (Ballroom and Expo Room)
- 1:00 PM – 2:00 PM **Afternoon Plenary Sessions**
- *Michael Graham*, Distinguished Professor, University of Wisconsin-Madison (Ballroom)
- *Heriberto Cabezas*, Senior Science Advisor, Sustainable Technology Division, U.S. EPA (Armour Dinning)
- 2:15 PM – 4:15 PM **Technical Sessions**
- *Fundamentals of Process Modeling and Equipment Design* (Ballroom)
- *Water and Wastewater: Treatment, and Management* (Armour Dinning)
- *Computational Methods in Biomedical Engineering* (Alumni Lounge)
- *Electrochemical Energy Conversion and Storage* (Herman Lounge)
- *Professional Development: Entrepreneurship Panel* (Expo Room)
- *Professional Development: Resume Workshop* (Armour Conference Room)
- *MRC 2016 Planning Meeting* (Room 006)
- 4:30 PM – 6:00 PM **Poster Session** (Gallery Lounge)
- 6:00 PM – 7:00 PM **AIChE Chicago March Dinner Meeting** (Ballroom)
- 7:00 PM – 8:00 PM **Dinner Keynote** (Ballroom)
- *June Wispelwey*, Executive Director, AIChE Global

AIChE Midwest Regional Conference Program at a Glance

Friday, March 13, 2015

- 7:30 AM - 10:00 AM **Continental Breakfast** (Gallery Lounge)
- 8:00 AM – 9:15 AM **Morning Keynote** (Ballroom)
- *Chris Gosling*, Director of Refining Development, UOP, A Honeywell Company
- 9:30 AM – 11:30 AM **Technical Sessions**
- *Refining Strategies for Maintaining High Production* (Ballroom)
- *Advances in Catalysis* (Armour Dinning)
- *Biomaterials* (Alumni Lounge)
- *Process Safety and Occupational Health* (Herman Lounge)
- *Advances in Optimization I* (Trustee Room / Room 010)
- *Professional Development: Mock Interviews* (Armour Conference Room)
- 11:30 AM – 1:00 PM **Lunch with High School Outreach Participants** (Ballroom and Expo Room)
- 1:00 PM – 2:00 PM **Afternoon Plenary Sessions**
- *Lonnie D. Shea*, Professor and Chair, Biomedical Engineering, University of Michigan (Ballroom)
- *Peter Lodal*, Group Leader, Plant Protection Technical Services, Eastman Chemical (Armour Dinning)
- 2:15 PM – 4:15 PM **Technical Sessions**
- *Refining Technology to Improve Feed Flexibility and Product Value* (Ballroom)
- *Catalysis for Chemicals Synthesis* (Armour Dinning)
- *Drug Delivery* (Alumni Lounge)
- *Power and Energy Systems* (Herman Lounge)
- *Advances in Optimization II* (Trustee Room / Room 010)
- *Professional Development: Life Skills* (Room 007)
- *MRC 2016 Planning Meeting* (Room 006)
- 4:15 PM – 6:00 PM **Closing Reception** (Ballroom)
- 4:30 PM – 5:30 PM **Closing Keynote** (Ballroom)
- *Henrik Rasmussen*, Vice President of Catalyst and Technology, Haldor Topsoe
- 6:00 PM – 8:00 PM **Young Professional Networking Social** (Off-Site)

AICHE Midwest Regional Conference Keynote and Plenary Speakers (Thursday)

Thursday Morning Keynote: 8:00 AM Thursday, March 12, 2015

C.J. Warner, Executive Vice President, Tesoro Corporation

Presentation Title: **Energy Evolution: How Engineering and Technology are Creating an Abundant Global Energy Portfolio**

Biographical Sketch: Cynthia (CJ) Warner is Executive Vice President, Strategy and Business Development for Tesoro Corporation. Ms. Warner joined Tesoro in 2014, bringing more than 30 years of experience in energy, oil refining and marketing to her role as leader of the Company's strategic growth initiatives.

Prior to Tesoro, Ms. Warner held executive leadership roles at several global energy companies. Most recently, she was Chairman and CEO of Sapphire Energy from 2012 to 2014, after joining as President in 2009, where she led the emerging biofuels company's ongoing technology development and transition to commercial-scale algae bio mass and renewable crude oil production. Prior to Sapphire Energy, Ms. Warner served as Group Vice President of Global Refining and Group Vice President of Health, Safety, Security, Environmental and Technology for British Petroleum (BP). Ms. Warner began her career as a chemical engineer at UOP, followed by several years in operational leadership roles at Amoco. She is a featured leader in the 2008 book 'Becoming a Resonant Leader: Develop Your Emotional Intelligence' (Harvard Business Press) and was named one of Fast Company's 100 most creative people in business in 2010. She is also a member of the National Petroleum Council and President Obama's National Clean Energy Policy advisory body.

Ms. Warner earned a Bachelor of Engineering degree in Chemical Engineering from Vanderbilt University and a Master of Business Administration degree from Illinois Institute of Technology



Thursday Plenary Session I: 1:00 PM Thursday, March 12, 2015

Heriberto Cabezas, Senior Science Advisor, U.S. EPA

Presentation Title: **Designing Supply Chains with the P-graph Methodology under Sustainability Considerations**

Biographical Sketch: Heriberto Cabezas is the Senior Science Advisor to the Sustainable Technology Division in the U.S. EPA Office of Research and Development (ORD). At the U.S. EPA he is responsible for the scientific oversight of the scientific research teams under the guidance of the division director. He is a former Acting Director (2008-2010) of the Sustainable Technology Division and organized and led (2000-2008) the Sustainable Environments Branch, a multidisciplinary research group of some seventeen scientists and engineers. He is also an Associate Professor in the Department of Computer Science and Systems Technology at the University of Pannonia

Cabezas is a recipient of the 1998 U.S. EPA Science Achievement Award in Engineering, the 2007 Distinguished Alumni Achievement Award from the New Jersey Institute of Technology, the 2011 Research Excellence Award in Sustainable Engineering from the AIChE, the ORD Sustainability Award



(team) at the U.S. EPA, and the 2013 Lawrence K. Cecil Award in Environmental Chemical Engineering from the AIChE. He is a Fellow of the AIChE and a Board Certified Member of the American Academy of Environmental Engineers and Scientists. He holds a PhD and MS from the University of Florida, a BS from the New Jersey Institute of Technology, all in chemical engineering, and is a decorated U.S. Navy veteran of the Vietnam Conflict.

Thursday Plenary Session II: 1:00 PM Thursday, March 12, 2015

Michael D. Graham, Distinguished Professor, University of Wisconsin-Madison

Presentation Title: ***Collide and Conquer: Flow-induced Segregation Phenomena in Blood and Other Multicomponent Suspensions***

Biographical Sketch: Michael D. Graham is the Vilas Distinguished Achievement Professor and Harvey D. Spangler Professor of Chemical and Biological Engineering at the University of Wisconsin-Madison. Professor Graham's research activities focus on theoretical and computational studies of the fluid dynamics of complex fluids. Recent interests include: the rheology and dynamics of polymer solutions and suspensions, especially under confinement; blood flow in the microcirculation, swimming microorganisms; multi-scale computational methods; and instabilities and turbulence in complex fluids. He is coauthor of a textbook "Modeling and Analysis Principles for Chemical and Biological Engineers".



Awards include Best Student Paper Award from the Environmental Division of AIChE in 1986, a CAREER Award from NSF in 1995, the François Frenkiel Award for Fluid Mechanics from the American Physical Society Division of Fluid Dynamics in 2004, Fellowship in the APS in 2011 and the Kellett Mid-Career Award at UW-Madison in 2012. He has presented many named and plenary lectures, including the 2013 Ronald F. Probstein Lecture in Engineering Science at MIT. He was an Associate Editor of the Journal of Fluid Mechanics from 2005-2012. Presently he is a member of the editorial board of Physical Review E and is Editor of the Journal of Non-Newtonian Fluid Mechanics. Graham received his B.S. in Chemical Engineering from the University of Dayton in 1986 and his PhD. from Cornell University in 1992.

Thursday Dinner Keynote: 7:00 PM Thursday, March 12, 2015

June Wispelwey, Executive Director, AIChE Global

Presentation Title: ***How My Career Led to AIChE***

Biographical Sketch: Before becoming the executive director of the American Institute of Chemical Engineers (AIChE), June served as executive director of the Society for Biological Engineering (SBE), overseeing its successful launch and growth. Prior to working with the Society for Biological Engineering, she served as vice president of marketing services at Aventis Behring and as director of performance chemicals business development at Lyondell. June earned a bachelor's degree in chemical engineering at Princeton University and a master's degree in chemical engineering at the University of Pennsylvania. Additionally, she completed Aventis' Executive Education Program at the Wharton School of Business in Philadelphia.



AIChE Midwest Regional Conference Keynote and Plenary Speakers (Friday)

Friday Morning Keynote: 8:00 AM Friday, March 13, 2015

Chris Gosling, *Director of Refining Technology Development, UOP/Honeywell*

Presentation Title: ***Refining Technology and Configuration for Future Fuels***

Biographical Sketch: *Chris Gosling is the Director of UOP's Refining Technology Development group that is responsible for the development of new Hydroprocessing, FCC, Gasoline, Heavy Oil and Renewable Energy technologies. Chris joined UOP in 1980 after graduating from Michigan Technological University with BS and MS degrees in Chemical Engineering. He has held various positions within UOP, working in wide variety of technologies in Research and Development, Technical Service and Product Line Management. He is a registered Professional Engineer in Michigan, holds 45 patents, and has published many technical papers.*



Friday Plenary Session I: 1:00 PM Friday, March 13, 2015

Peter Lodal, *Technical Fellow, Eastman Chemical Company*

Presentation: ***Do We Really Need More Process Safety Leadership?***

Biographical Sketch: *Peter Lodal is a technical fellow and group leader of the Plant Protection Technical Services group at Eastman Chemical's Tennessee Operations site in Kingsport, TN. With over 20 of experience in process safety and loss prevention, he is Eastman Chemical Company's representative to the Center for Chemical Process Safety (CCPS) Technical Steering Committee. Pete chairs the Process Safety Committee for the American Chemistry Council (ACC) and serves on the International Editorial Board for the Journal of Loss Prevention in the Process Industries.*

Lodal is a Fellow of the American Institute of Chemical Engineers (AIChE) and a Fellow of the Center for Chemical Process Safety (CCPS). He was awarded the Outstanding Engineer of the year in 2004 by the Upper East Tennessee Chapter of the Tennessee Society of Professional Engineers. He was the 2010 Chair of AIChE's Safety and Health division. He was also the 2013 Trevor Kletz Merit Award Winner, given by the Mary Kay O'Connor Process Safety Center at Texas A&M University. He holds BS (1976) and MS (1977) degrees in Chemical Engineering from Purdue University.



Friday Plenary Session II: 1:00 PM Friday, March 13, 2015

Lonnie D. Shea, *Professor and Chair of Biomedical Engineering, University of Michigan*

Presentation Title: **Systems Tissue Engineering**

Biographical Sketch: *Lonnie D. Shea is professor and chair in the Department of Biomedical Engineering at the University of Michigan, with a joint appointment in the Department of Chemical Engineering. He received his BS and MS degrees at Case Western Reserve University in Chemical Engineering and his PhD in Chemical Engineering and Scientific Computing at the University of Michigan. He joined the faculty of Northwestern University in 1999 within the Department of Chemical and Biological Engineering, and retains an appointment in that department as well as in Obstetrics and Gynecology at Feinberg School of Medicine.*



The Shea research group works at the interface of tissue engineering, gene therapy, and drug delivery. He received an NSF CAREER Award in 2000, which helped start the work on developing new technologies based on combining biomaterials and gene/drug delivery. The overall objective is to create controllable microenvironments for directing or molecularly dissecting tissue growth. These systems are being applied to clinical problems such as ovarian follicle maturation for treating infertility, islet transplantation for diabetes therapies, nerve regeneration for treating paralysis. More recently, his research has moved into cancer diagnostics, autoimmune disease, and systems biology applied to regenerative medicine. In addition to his teaching and research commitments, he was director of the NIH Biotechnology Training Grant at Northwestern University. Dr. Shea is a fellow of the American Institute of Medical and Biological Engineering, and is a member of the editorial boards for Molecular Therapy, Biotechnology and Bioengineering, and Drug Delivery and Translational Research.

Closing Keynote: 4:30 PM Friday, March 13, 2015

Henrik Rasmussen, *Vice President of Catalyst and Technology, Haldor Topsoe*

Presentation Title: **The Shale Gas revolution in the US**

Biographical Sketch: *Henrik Rasmussen graduated from the University of Copenhagen in 1989 with a degree in chemical engineering before relocating to the United States in 1991. He has worked at Haldor Topsoe for more than 25 years and has held a number of technical and management positions for all of Topsoe's business units. Mr. Rasmussen is currently the Vice President of Catalyst and Technology and, in that capacity, is responsible for the catalyst and license technology business for the U.S., Canada, and the Caribbean.*



AIChE Midwest Regional Conference
Session Presentations
Thursday, March 12, 2015

Morning Keynote Session

Thursday, March 12, 2015 (Ballroom)

8:00 AM Welcoming Remarks

Azita Ahmadzadeh (UOP/Honeywell)

8:10 AM Keynote Introduction

John Anderson (Illinois Institute of Technology)

8:20 AM Energy Evolution: How Engineering and Technology are Creating the an Abundant Global Energy Portfolio

C.J. Warner (Tesoro Corporation)

Refinery Integrity Management

Thursday, March 12, 2015 (Ballroom, **ThA1**)

Chair: *Jerry Wilks (CITGO Petroleum)*

9:30 AM High Temperature Damage Mechanism in Refinery Environments (ThA1a)

Bernard Schulze (Stress Engineering Services)

9:55 AM CFD Investigation of a Hydrogen Reformer Furnace for Improved Flow Distribution (ThA1b)

Bin Wu, Chenn Q. Zhou, Armin Silaen (Purdue University Calumet)

10:20 AM Analysis of Refinery Equipment to Improve Unit Start-ups and Shut-Downs (ThA1c)

Jerry Wilks (CITGO Petroleum)

10:45 AM Application of Metal Oxides to Alleviate Corrosion from Chlorides (ThA1d)

Hans-Christoph Schwarzer, Axel Düker (Clariant)

Advances in Bioremediation of Chemical

Contaminants

Thursday, March 12, 2015 (Armour Dinning, **ThA2**)

Chair: *Jarad L. Champion (Geosyntec),*

Co-chair: *Pahola Thathiana Benavides (VRI-Custom)*

9:30 AM Advances in 1,2,3-TCP Remediation in Groundwater via Biological Reduction (ThA2a)

Melissa Schmitt, Eric Sucomel, Sandra Dworatzek, Jeff Roberts, Phil Dennis (Geosyntec Consultants)

9:55 AM Using Correlations to find Causations: a Statistical Model to Direct PCB Bioremediation Studies (ThA2b)

Amanda Hughes (Geosyntec Consultants) Mitch Small, Jeanne VanBriesen (Carnegie Mellon University)

10:20 AM Bioremediation at Low pH - Emerging Tools and Approaches for Chlorinated Solvent Sites (ThA2c)

Phil Dennis, Sandra Dworatzek, Jeff Roberts, Peter Dollar (SiREM)

10:45 AM In-situ Bioremediation and ZVI Injections for Source Abatement, Beneath an Active Manufacturing Facility (ThA2d)

Chriso Petropoulou, Valerie Bosscher, J. Neil Couch, Sean Carbonaro, Mary DeFlaun (Geosyntec Consultants), Jeff Roberts (SiREM)

Advances in Pharmaceuticals

Thursday, March 12, 2015 (Alumni Lounge, **ThA3**)

Chair: *Zoltan K. Nagy (Purdue University)*

9:30 AM Decoupling of Spherical Crystallization Mechanisms in a Two-Stage MSMPR (ThA3a)

Ramon Peña, Zoltan K. Nagy (Purdue University)

9:50 AM Combined Product and Process Design of a Multi-Stage Mixed-Suspension-Mixed-Product Removal (MSMPR) Cooling Crystallization System under Dissolution, Growth and Nucleation Mechanisms (ThA3b)

David Acevedo, Zoltan K. Nagy (Purdue University)

10:10 AM Advanced Control Approaches for Combined Cooling/Antisolvent Crystallization in Continuous Mixed Suspension Mixed Product Removal Cascade Crystallizers (ThA3c)

Yang Yang, Zoltan K. Nagy (Purdue University)

10:30 AM Closed-Loop Control for the Feeder and Blender Unit Operations into the Continuous-Tablet Manufacturing Process (ThA3d)

Mariana Moreno, Zoltan K. Nagy, Gintaras V. Reklaitis, Arun Giridhar (Purdue University)

10:50 AM Engineered Biosensor Proteins for Remote Control of Engineered Cell-Based Therapies (ThA3e)

Kelly Schwarz, Nichole Daringer, Rachel Dudek, Joshua Leonard (Northwestern University)

11:10 AM **Development and Control of a Drop-on-Demand Manufacturing System for the Production of Melt-based Pharmaceuticals** (ThA3f)
Elcin Icten, Arun Giridhar, Zoltan K. Nagy, Gintaras Reklaitis (Purdue University)

Renewable Energy Sources and Systems

Thursday, March 12, 2015 (Herman Lounge, **ThA4**)

Chair: *Jordan Ciezobka* (Gas Technology Institute)

9:30 AM **Gas Fermentation of Carbon Residues to Fuels and Chemicals** (ThA4a)

Rachel Brenck (LanzaTech)

9:50 AM **Techno-Economic Analyses and Life Cycle Assessment of Two Stage Fast Pyrolysis for Bio-oil Production from Pine Wood** (ThA4b)

Olumide Winjobi, David Shonnard, Wen Zhou, Ezra Bar Ziv (Michigan Technological University)

10:10 AM **Opportunities and Challenges for Energy-Intensive Chemicals: Emerging Technology Review** (ThA4c)

Yuan Yao (Northwestern University), *Diane Graziano* (Argonne National Lab), *Matthew Riddel* (Argonne National Lab), *Eric Masanet* (Northwestern University)

10:30 AM **Advanced Electrocatalysts for Fuel Cells** (ThA4d)

Vojislav Stamenkovic, Dongguo Li, Yijin Kang, Dusan Strmcnik, Nenad Markovic (Argonne National Lab)

10:50 AM **Optimal Closed-loop Design of Grid Scale Energy Storage Systems** (ThA4e)

Oluwasanmi Adeodu, Donald Chmielewski (Illinois Institute of Technology)

11:10 AM **Efficient Solar Thermal Integrated Power and Chemical Production Cycles for Uninterrupted Power Supply** (ThA4f)

Emre Gençer, Mohit Tawarmalani, Rakesh Agrawal (Purdue University)

Professional Development: YP Engineering 101

Thursday, March 12, 2015 (Armour Conf Room, **ThA5**)

Chair: *Janet Werner* (Sensient)

9:30 AM **Mixing Fundamentals and High Shear Mixing Benefits** (ThA5a)

Don Mansfield, Brian Martin (Silverson High Shear Mixers)

10:00 AM **Intro to Centrifugal Pumps** (ThA5b)

Thomas C. Wood (Flowserve)

10:30 AM **English 101: Email, Meetings, and Internet at Work** (ThA5c)

Dennis O'Brien (Jacobs Consultancy)

11:00 AM **Meeting Etiquette: Basics of Project Communication** (ThA5d)

Annette A Johnston (Abbott Laboratories)

Thursday Plenary Session I

Thursday, March 12, 2015 (Armour Dinning)

1:00 PM **Plenary Introduction**

Urmila Diwekar (Vishwamitra Research Institute)

1:10 PM **Designing Supply Chains with the P-graph Methodology under Sustainability Considerations**

Heriberto Cabezas (Senior Science Advisor, Sustainable Technology Division, U.S. EPA)

Thursday Plenary Session II

Thursday, March 12, 2015 (Ballroom)

1:00 PM **Plenary Introduction**

David Venerus (Illinois Institute of Technology)

1:10 PM **Collide and Conquer: Flow-induced Segregation Phenomena in Blood and Other Multicomponent Suspensions**

Michael Graham (Distinguished Professor, University of Wisconsin-Madison)

Fundamentals of Process Modeling and Equipment Design

Thursday, March 12, 2015 (Ballroom, **ThB1**)

Chair: *Rajeswar Gattupalli* (UOP/Honeywell)

Co-chair: *Adam Kanyuh* (UOP/Honeywell)

2:15 PM **Molecular Dynamics Simulation of Gas Solubility in n-Alkanes and n-Alcohols** (ThB1a)

Kevin R. Hinkle (UIC), *Paul M. Mathias* (Fluor), *Sohail Murad* (Illinois Institute of Technology)

2:35 PM **Accuracy of Predictive Thermodynamic Models for Modeling Difficult Separation Processes** (ThB1b)

Eric Cheuget (UOP/Honeywell)

2:55 PM **Systematic Analysis and Convenient Prediction of Steady State Multiplicity Patterns** (ThB1c)

Satish J. Parulekar (Illinois Institute of Technology)

3:15 PM **Computational Fluid Dynamics (CFD) for Process and Equipment Design and Development** (ThB1d)

Quan Yuan, Reza Mostofi-Ashtiani, Hadjira Iddir (UOP/Honeywell)

3:35 PM **Small-Scale LNGP with Modular SMR Technology** (ThB1e)

Trevor Smith (UOP/Honeywell)

3:55 PM **A New Slurry Bubble Column Reactor for Diesel Fuel** (ThB1f)

Dimitri Gidaspow, Yuting He, Vishak Chandra (Illinois Institute of Technology)

Water and Wastewater: Treatment and Management

Thursday, March 12, 2015 (Armour Dinning, **ThB2**)

Chair: *Urmila Diwekar* (VRI-Custom)

2:15 PM **Mercury Removal from Industrial Aqueous Streams** (ThB2a)

Pravan Pappu, Andrea Foster, Rachel Mansfield (Johnson Matthey)

2:35 PM **Optimal Design of Adsorbents for NORM Removal from Produced Water in Natural Gas Fracking – Part I: Group Contribution Method for Adsorption** (ThB2b)

Pahola Thathiana Benavides, Urmila Diwekar, Berhane Gebreslassie (VRI-Custom)

2:55 PM **Optimal Design of Adsorbents for NORM Removal from Produced Water in Natural Gas Fracking – Part 2: CAMD for Adsorption of Radium and Barium** (ThB2c)

Pahola Thathiana Benavides, Urmila Diwekar, Berhane Gebreslassie (VRI-Custom)

3:15 PM **Life Cycle Mass Flow Analysis of Water Demand, Produced Water Output and Solid Wastes Associated with Shale Gas Development Areas: A First Step in Estimating Impacts** (ThB2d)

Tom Hays (Gas Technology Institute)

3:35 PM **Optimization Application in Water Distribution Networks Using Embedded Hydraulic Models** (ThB2e)

Arpan Seth, Carl D. Laird (Purdue University)

Computational Methods in Biomedical Engineering

Thursday, March 12, 2015 (Alumni Lounge, **ThB3**)

Chair: *Ali Cinar* (Illinois Institute of Technology)

2:15 PM **Surface-Functionalized Nanoparticle Permeation Triggers Lipid Displacement and Ion and Water Leakage** (ThB3a)

Priyanka Oroskar, Sohail Murad, Cynthia Jameson (University of Illinois at Chicago)

2:30 PM **Stochastic Optimal Control for Prediction of Robust Drug Dosing Policies in Superovulation Stage of In-Vitro Fertilization** (ThB3b)

Kirti M. Yenkie, Urmila Diwekar (VRI-CUSTOM and UIC)

2:45 PM **Energy Expenditure Modeling and Its Use in Glucose Concentration Predictions** (ThB3c)

Thiago Marques Luz Paulino, Ali Cinar, Kamuran Turksoy (Illinois Institute of Technology)

3:00 PM **MINEng Computationally Predicted Enzyme Promiscuity Products for Untargeted Metabolomics** (ThB3d)

James Jeffryes (Northwestern University), *Ric Colasanti* (Argonne National Lab), *Keith Tyo* (Northwestern University), *Christopher Henry* (Argonne National Lab)

3:15 PM **Meal Detection Based on Qualitative Representation of Continuous Glucose Monitor Measurements** (ThB3e)

Sediqeh Samadi, Kamuran Turksoy, Ali Cinar (Illinois Institute of Technology)

3:30 PM **Parameter Estimation in Cellular Systems Modeled as Stochastic Differential Equations** (ThB3f)

Kirti M. Yenkie, Urmila Diwekar, Andreas Linninger (UIC)

3:45 PM **Parameter Estimation of Spatiotemporal Infectious Disease Models Using Nonlinear Dynamic Optimization** (ThB3g)

Michael Bynum, Carl Laird (Purdue University)

4:00 PM **A Hybrid Kinetic Model for Synthesis of Monoclonal Antibodies by Hybridoma Cells** (ThB3h)

Denizhan Yilmaz, Satish J. Parulekar, Ali Cinar (Illinois Institute of Technology)

Electrochemical Energy Conversion and Storage

Thursday, March 12, 2015 (Herman Lounge, **ThB4**)

Chair: *Nancy N. Kariuki* (Argonne National Lab)

2:15 PM **The effects of Structure and Composition of Microporous Layer on Performance in Electrochemical Reduction of CO₂** (ThB4a)

Byoungsu Kim, Febrian Hillman, Paul J.A Kenis (University of Illinois at Urbana-Champaign)

2:35 PM **High-k Laminated Polymer Composites with Extremely Low Dielectric Loss for Embedded Capacitors** (ThB4b)

Binghao Wang (Northwestern University), *Aijuan Gu* (Soochow University), *Tobin J. Marks, Antonio Facchetti* (Northwestern University)

2:55 PM **Monolayer (Hydroxy)oxide-Metal Bifunctional Electrocatalysts for Hydrogen**

Evolution Reaction: A First-Principles Perspective
(ThB4c)

Zhenhua Zeng, Joseph Kubal, Jeff Greeley (Purdue University)

3:15 PM **Probing the Synthesis and Structure of Li_5FeO_4 (LFO) Cathodes in Li-ion Cells** (ThB4d)

Chi-Kai Lin, Xiaoping Wang, Michael Krumpelt, Christopher Johnson (Argonne National Lab)

3:35 PM **GLAD-SAD Pt-Ni alloy/Ni Nanorod Electrocatalysts as Highly Active Oxygen Reduction Reaction** (ThB4e)

Nancy N. Kariuki (Argonne National Lab), *Mehmet F. Cansizoglu, Mahbuba Begum, Mesut Yurukcu, Fatma M. Yurtsever, Tansel Karabacak* (University of Arkansas at Little Rock), *Deborah J. Myers* (Argonne National Lab)

3:55 PM **Non-Carbon Catalyst Supports for Polymer Electrolyte Fuel Cells** (ThB4f)

Xiaoping Wang, Tammi Nowicki, Nancy Kariuki, Debbie Myers, Chi-Kai Lin, Yang Ren (Argonne National Lab)

Professional Development: Entrepreneurship Panel

Thursday, March 12, 2015 (Expo Room, ThB5)

Chair: *Nik Rokop* (Illinois Institute of Technology)

2:15 PM **Panel on Entrepreneurship**

Said Al-Hallaj (AllCell), *Bonnie Haferkamp* (Illinois Institute of Technology), *Raja Krishnan* (Technology Transfer Consultant), *Jason Zielke* (LocusView)

Professional Development: Resume Workshop

Thursday, March 12, 2015 (Armour Conf Room, ThB6)

Chair: *Janet Werner* (Sensient)

2:15 PM **Panel of Resume Experts**

Kamara Jackson (Illinois Institute of Technology), *Janet Werner* (Sensient), *Sara Dell* (Illinois Institute of Technology), *Julie Gruhn* (UOP/Honeywell)

MRC 2016 Planning Meeting

Thursday, March 12, 2015 (Room 006, ThB7)

Chair: *Donald Chmielewski* (Illinois Institute of Technology)

2:30 PM **Program Planning for MRC 2016**

Donald Chmielewski (Illinois Institute of Technology)

Poster Session

Thursday, March 12, 2015 (Gallery Lounge)

Chair: *Satish Parulekar* (Illinois Institute of Technology)
Co-Chair: *Belinda Akpa* (University of Illinois at Chicago)

4:30 PM **Poster Session**

Poster titles and abstracts to be distributed on site

Local Section Dinner Program

Thursday, March 12, 2015 (Ballroom)

6:40 PM **Local Section Announcements**

Azita Ahmadzadeh (UOP/Honeywell)

6:50 PM **Thiele Award Presentation to Alan Zagoria**

James Simnick (BP)

7:00 PM **Keynote Introduction**

Dennis O'Brien (Jacobs Consultancy)

7:10 PM **How My Career Led to AIChE**

June Wispelwey (Executive Director, AIChE Global)

AIChE Midwest Regional Conference

Session Presentations

Friday, March 13, 2015

Morning Keynote Session

Friday, March 13, 2015 (Ballroom)

8:00 AM **Recognition for Volunteers from the GAC Chair**

Jerry Wilks (CITGO Petroleum)

8:10 AM **Keynote Introduction**

Paolo Palmas (UOP/Honeywell)

8:20 AM **Refining Technology and Configuration for Future Fuels**

Chris Gosling (UOP/Honeywell)

Refining Strategies for Maintaining High Production

Friday, March 13, 2015 (Ballroom, FrA1)

Chair: *Martin Gonzalez* (BP)

9:30 AM **Relieving Unit Constraints with My First DMC Application** (FrA1a)

Carl Towner (BP)

9:55 AM **Oxygen for Improved Refinery Utilization** (FrA1b)

David Lenhart (Praxair), *John Scalise* (Praxair)

10:20 AM **Refinery Hydrogen Dynamics – Impact of Tight Oil and Shale Gas** (FrA1c)

Ken Chlapik (Johnson Matthey)

10:45 AM **Safer and Smarter Catalyst Sulfiding** (FrA1d)

Randy Alexander, Mike Robinson (Reactor Resources)

Advances in Catalysis

Friday, March 13, 2015 (Armour Dinning, FrA2)

Chair: *Christopher L. Marshall* (Argonne National Lab)

Co-Chair: *Justin Notestein* (Northwestern University)

9:30 AM **Fundamental Mechanistic Studies of Formic Acid Decomposition on Pd: Structure Sensitivity and Surface Coverage Effects** (FrA2a)

Sha Li (University of Wisconsin Madison), *Jessica Scaranto* (SABIC), *Srinivas Rangarajan* and *Manos Mavrikakis* (University of Wisconsin Madison)

9:50 AM **Synthesis and Evaluation of Highly Dispersed FeOx-CeO₂ Catalysts for NO_x Reduction** (FrA2b)

Justin Notestein, Dario Prieto-Centurion, and Louisa Savereide (Northwestern University), *Charles Roberts and Paul Fanson* (Toyota)

10:10 AM **Systematic Study of Support Effects on Selective Hydrogenation of Acrolein** (FrA2c)

Payoli Aich (UIC), *Haojuan Wei* (UIC), *Christopher L. Marshall* and *Jeffrey T. Miller* (Argonne National Lab), *Randall J. Meyer* (UIC)

10:30 AM **ALD Overcoating as a Means for Improving Catalyst Selectivity and Stability** (FrA2d)

Christopher L. Marshall (Argonne National Lab), *Hongbo Zhang* (Argonne National Lab), *Peter C. Stair* (Northwestern University), *Jeffrey W. Elam* (Argonne National Lab), *Brandon O'Neill* (University of Wisconsin), *James A. Dumesic* (University of Wisconsin)

10:50 AM **Impact of Spatial Segregation in Catalytic Reactors – Two Identical Reactors with One-Way and Two-Way Interaction** (FrA2e)

Satish J. Parulekar (Illinois Institute of Technology)

11:10 AM **An Experimental and Theoretical Study of Glycerol Selective Oxidation to 1,3-Dihydroxyacetone via Bimetallic Platinum-Bismuth Catalysts** (FrA2f)

Yang Xiao, Zhi-jian Zhao, Jeffrey Greeley, and Arvind Varma (Purdue University)

Biomaterials

Friday, March 13, 2015 (Alumni Lounge, FrA3)

Chair: *Nancy W. Karuri* (Illinois Institute of Technology)

9:30 AM **Agent-Based Modeling of Concurrent Biomaterial Scaffold Degradation and Vascularization** (FrA3a)

Chenlin Lu (Illinois Institute of Technology), *Hamidreza Mehdizadeh* (Pfizer), *Elif Seyma Bayrak* (Amgen), *Sami Somo, Eric M. Brey, Ali Cinar* (Illinois Institute of Technology)

9:45 AM **Proteolysis of Decellularized Extracellular Matrices Generates a Significant Amount of Fibronectin Fragments** (FrA3b)

Anand Ramanathan, Nancy W. Karuri (Illinois Institute of Technology)

10:00 AM **Substrate Stiffness Influence on Adipose Tissue Expansion and Function** (FrA3c)

Marcella Vaicik (Illinois Institute of Technology), *Ronald Cohen* (University of Chicago), *Jose Rios*,

Georgia Papavasiliou, and Eric M. Brey (Illinois Institute of Technology)

10:15 AM **Agent-Based Simulation of Growth Factor Releasing Biomaterials** (FrA3d)

Nan Xiao, Elif S. Bayrak, Banu Akar, Hamidreza Mehdizadeh, Sami Somo, Eric M. Brey, Ali Cinar (Illinois Institute of Technology)

10:30 PM **Ceramic-Hydrogel Composites Augment Bone Regeneration in a Rodent Critical Size Defect Model** (FrA3e)

Banu Akar (Illinois Institute of Technology), *Shu-Wei Kao* (Chang Gung Memorial Hospital), *Katerina Stojkova* (Illinois Institute of Technology), *Ming-Huei Cheng* (Chang Gung Memorial Hospital), *Eric M. Brey* (Illinois Institute of Technology)

10:45 AM **Gradient Scaffolds for Vascularized Tissue Formation** (FrA3f)

Yusheng He, Georgia Papavasiliou (Illinois Institute of Technology)

11:00 AM **Fibronectin Matrix Degradation by α -Chymotrypsin** (FrA3g)

Xue Geng, Yaozhu Leng (Illinois Institute of Technology)

11:15 AM **Cell Deprivation: Nutrient Limitation and Gene Knockouts of Escherichia Coli towards Enhancing Non-Growth Metabolism for Metabolic Engineering Purposes** (FrA3h)

Will Bothfeld, Jennifer Greene, Divya Tikkavarapu, Grace Kapov, Keith Tyo (Northwestern University)

Process Safety and Occupational Health

Friday, March 13, 2015 (Herman Lounge, **FrA4**)

Chair: *Brenton L. Cox* (Exponent)

Co-Chair: *Janet A. Grezlik* (PSRG Inc.)

9:30 AM **Lessons Learned from PSM Auditing and OSHA's Plans for Change** (FrA4a)

Bob Weber (PSRG Inc)

9:50 AM **Hazards Inherent to Batch Processing: Lessons Learned from Case Studies** (FrA4b)

Brenton L. Cox, Sean J. Dee, Andrew R. Carpenter, Russell A. Ogle (Exponent)

10:10 AM **Ignition of Flammable Vapors in Partially Filled Containers** (FrA4c)

Sean J. Dee, Brenton L. Cox, Russell A. Ogle (Exponent)

10:30 AM **Discrepancies in Methods for the Predicting the Explosion Energy of BLEVEs** (FrA4d)

Ronald Pape, Amy Richards, Michael Hanks (Engineering Systems Inc.)

10:50 AM **Scaling Analysis for Confined Dust Flame Propagation** (FrA4e)

Russell A. Ogle, Brenton L. Cox, Sean J. Dee (Exponent)

11:10 AM **Managing Change – Hurdles of the Past and Innovation for the Future** (FrA4f)

Oleg Yazvin and Eric Allen (Environmental Intellect)

Advances in Optimization I

Friday, March 13, 2015 (Trustee Room / Room 010, **FrA5**)

Chair: *Carl Laird* (Purdue University)

9:30 AM **Large-Scale Multi-Objective Multi-Stakeholder Optimization** (FrA5a)

Victor Zavala (Argonne National Lab)

9:50 AM **Efficient Ant Colony Optimization (EACO) Algorithm for Large Scale Optimization Problems** (FrA5b)

Berhane H. Gebreslassie and Urmila M. Diwekar (Vishwamitra Research Institute)

10:10 AM **Multi-agent Optimization Framework to Solve Large Scale Process System Engineering Problems** (FrA5c)

Berhane H. Gebreslassie and Urmila M. Diwekar (Vishwamitra Research Institute)

10:30 AM **Clustering-Based Preconditioning for Stochastic Programs** (FrA5d)

Yankai Cao and Carl Laird (Purdue University), *Victor Zavala* (Argonne National Lab)

10:50 AM **Globally Optimal Sensor Network Design Revisited: Application of the Generalized Bender Decomposition** (FrA5e)

Jin Zhang, Donald J. Chmielewski (Illinois Institute of Technology)

Professional Development: Mock Interviews

Thursday, March 13, 2015 (Armour Conf Room, **FrA6**)

Chair: *Julie Gruhn* (UOP/Honeywell)

9:30 AM **Panel of Interview Experts**

Kamara Jackson (Illinois Institute of Technology), *Janet Werner* (*Sensient*), *Sara Dell* (Illinois Institute of Technology), *Julie Gruhn* (UOP/Honeywell)

Friday Plenary Session I

Friday, March 13, 2015 (Armour Dinning)

1:00 PM **Plenary Introduction**

Trey Morrison (Exponent)

1:10 PM **Do We Really Need More Process Safety Leadership?**

Peter Lodal (Technical Fellow, Eastman Chemical Company)

Friday Plenary Session II

Friday, March 13, 2015 (Ballroom)

1:00 PM Plenary Introduction

Georgia Papavasiliou (Illinois Institute of Technology)

1:10 PM Systems Tissue Engineering

Lonnie D. Shea (Professor and Chair of Biomedical Engineering, University of Michigan)

Refining Technology to Improve Feed Flexibility and Product Value

Friday, March 13, 2015 (Ballroom, FrB1)

Chair: *Paolo Palmas* (UOP/Honeywell)

2:15 PM Shale Oil Processing Challenges: from the Reservoir to the Refinery (FrB1a)

Carl E. Weaver (Baker Hughes Inc)

2:35 PM Turning a Tier 3 Profit (FrB1b)

Jame Esteban (Criterion Catalysts and Technologies)

2:55 PM Tailoring Hydrocarbon Product Properties – Simple Solutions, Challenges, Limits – How to Find the Right Tools (FrB1c)

Rainer Rakoczy, Dieter Himsel (Clariant)

3:15 PM Innovative Process Changes for Improved LPG and Hydrogen Recovery in Platforming™ Process (FrB1d)

Robert Tsai, William Yanez, Frank (Xin X.) Zhu (UOP/Honeywell)

3:35 PM Refinery Forensics - Using Microscopy and Microanalysis in Refinery Trouble Shooting and Problem Solving (FrB1d)

Bradley Huggins (North Twin Microscopy Inc.)

Catalysis for Chemicals Synthesis

Friday, March 13, 2015 (Armour Dinning, FrB2)

Chair: *Michael Caracotsios* (UOP/Honeywell)

2:15 PM Controlling Au Particle Sintering During the Hydrochlorination of Acetylene Using Core-Shell Bimetals (FrB2a)

Kerry C. O'Connell, John R. Monnier, John Regalbutto (University of South Carolina)

2:35 PM Vapor phase Ethanol Carbonylation over Supported Rhodium Catalysts (FrB2b)

Sara Yacob and Sunyong Park (Northwestern University), *Beata Kiloa and David Barton* (Dow Chemical), *Justin Notestein* (Northwestern University)

2:55 PM Counting Active and Selective Sites on Niobia-Silica Catalysts for Alkene Epoxidation with H₂O₂ (FrB2c)

Nicholas Thornburg, Justin Notestein (Northwestern University)

3:15 PM Ethylene Carbonylation by Molybdenum Carbonyl Catalysts (FrB2d)

Chieh-Chao Yang (Northwestern University), *Beata Kilos and David Barton* (Dow Chemical), *Eric Weitz and Justin Notestein* (Northwestern University)

3:35 PM Effects of Solvent and Substituents on the Kinetics of Di-Olefin Epoxidation Catalyzed by Fe-porphyrin Complexes (FrB2e)

Ying Yu, Linda J. Broadbelt (Northwestern University)

3:55 PM Gas-Phase Dimerization of Ethylene under Mild Conditions Catalyzed by MOF Materials Containing Ni(II) Bipyridine Complexes (FrB2f)

Sherzod T. Madrahimov, SonBinh T. Nguyen (Northwestern University)

Drug Delivery

Friday, March 13, 2015 (Alumni Lounge, FrB3)

Chair: *Georgia Papavasiliou* (Illinois Institute of Technology)

2:15 PM A Controlled and Extended Drug Delivery System to Treat Posterior Segment Eye Diseases (FrB3a)

Christian Osswald, Jennifer J. Kang-Mieler (Illinois Institute of Technology)

2:35 PM Improved Induction of Apoptosis by Bortezomib loaded in Liposomal Nanocarriers: A Comparison between Cationic and Ceramide Liposomes (FrB3b)

Medha Joshi, Gabriel Park, Jennifer Pichlik, Annette Gilchrist (Midwestern University)

2:55 PM Engineering Exosomes as Therapeutic Delivery Vehicles (FrB3c)

Michelle E. Hung, Joshua N. Leonard (Northwestern University)

3:15 PM "Shake-n-Incubate": Examining the Effects of Orbital Shaking on Iron Oxide Nanoparticle Uptake for Stem Cell Labeling (FrB3d)

Nicholas E. Clay (University of Illinois Urbana-Champaign)

3:35 PM Controlled Vancomycin Release from a Biodegradable Hydrogel Ocular Drug Delivery System (FrB3e)

Emily Dosmar, Jennifer J. Kang-Mieler (Illinois Institute of Technology)

3:55 PM Sustained Delivery of a VEGF Mimetic Peptide for Scaffold Neovascularization (FrB3f)

Daniel A. Young, Georgia Papavasiliou (Illinois Institute of Technology)

Power and Energy Systems

Friday, March 13, 2015 (Herman Lounge, **FrB4**)

Chair: *William Ryan* (University of Illinois at Chicago)

2:15 PM **Promise Kept** (FrB4a)

Richard Meyer (American Gas Association)

2:35 PM **Generation IV Sodium Cooled Fast Breeder Reactors** (FrB4b)

Emmilyn Riley (University of Illinois at Chicago)

2:55 PM **Solid Oxide Fuel Cells for Energy Production, Conversion and Storage** (FrB4c)

Rick Dombrowski (University of Illinois at Chicago)

3:15 PM **Movable Bulb Turbine for Low Head Hydropower** (FrB4d)

Nikolay Popov (University of Illinois at Chicago)

3:35 PM **Business Model of Leasing Photovoltaic Solar Systems** (FrB4e)

Aidan Gilbert (University of Illinois at Chicago)

3:55 PM **Multiphase CFD and its application in precombustion CO₂ capture processes** (FrB4f)

Emad Ghadirian Hoseinabadi, Shahin Zarghami, Hamid Arastoopour, Javad Abbasian (Illinois Institute of Technology)

Advances in Optimization II

Friday, March 13, 2015 (Trustee Room / Room 010, **FrB5**)

Chair: *Fouad Teymour* (Illinois Institute of Technology)

Co-Chair: *Mustafa Cagdas Ozturk* (Illinois Institute of Technology)

2:15 PM **Optimal Sensor Placement under Uncertainty in Water Network System with Better Optimization of Non-Linear Uncertain Systems (BONUS) Algorithm** (FrB5a)

Rajib Mukherjee, Urmila M. Diwekar (Vishwamitra Research Institute)

2:35 PM **Controller Performance Assessment for Artificial Pancreas** (FrB5b)

Jianyuan Feng, Kamuran Turksoy, Ali Cinar (Illinois Institute of Technology)

2:55 PM **Optimization of Air Usage in Activated Sludge Processes** (FrB5c)

Mustafa Cagdas Ozturk, Fernando Martin Serrat, Fouad Teymour (Illinois Institute of Technology)

3:15 PM **Optimization Framework for MINLP Problems with Pyomo: Applications in Infectious Disease Parameter Estimation** (FrB5d)

Jianfeng Liu, Carl D. Laird (Purdue University)

3:35 PM **Selecting Optimum and Ideal Energized Fluids for Natural Gas Fracking** (FrB5e)

Urmila Diwekar (Vishwamitra Research Institute)

Professional Development: Life Skills

Friday, March 13, 2015 (Room 007, **FrB6**)

Chair: *Julie Gruhn* (UOP/Honeywell)

2:15 PM **A Career in Chemical Engineering** (FrB6b)

Pat Shannon (Middough)

2:45 PM **Intro to Financial Planning** (FrB6a)

John Dulay (Raymond James)

3:15 PM **How to Set Your Career Goals** (FrB6c)

Kamara Jackson (Illinois Institute of Technology)

MRC 2016 Planning Meeting

Friday, March 13, 2015 (Room 006, **FrB7**)

Chair: *Donald Chmielewski* (Illinois Institute of Technology)

2:30 PM **Program Planning for MRC 2016**

Donald Chmielewski (Illinois Institute of Technology)

3:00 PM **General Arrangements Planning for MRC 2016**

Jerry Wilks (Citgo)

Closing Keynote

Friday, March 13, 2015 (Ballroom)

4:30 PM **Keynote Introduction**

Martin R Gonzalez (BP)

4:40 PM **The Shale Gas revolution in the US**

Henrik Rasmussen (Vice President of Catalyst and Technology, Haldor Topsoe)

AIChE Midwest Regional Conference

Keynote and Plenary Abstracts

Thursday Morning Keynote Session

Thursday, March 12, 2015 (Ballroom)

8:00 AM **Conference Welcoming Remarks**

Azita Ahmadzadeh (UOP/Honeywell)

8:10 AM **Keynote Introduction**

John Anderson (Illinois Institute of Technology)

8:20 AM **Energy Evolution: How Engineering and Technology are Creating an Abundant Global Energy Portfolio**

C.J. Warner (Tesoro Corporation)

Thursday Plenary Session I

Thursday, March 12, 2015 (Armour Dinning)

1:00 PM **Plenary Introduction**

Urmila Diwekar (Vishwamitra Research Institute)

1:10 PM **Designing Supply Chains with the P-graph**

Methodology under Sustainability Considerations

Heriberto Cabezas^{1,2}, *István Heckl*¹, *Leisha Vance*², *Botond Bertok*¹, *Ferenc Friedler*¹ (¹Department of Computer Science and Systems Technology, University of Pannonia, Hungary, ²Office of Research and Development, U.S. Environmental Protection Agency)

The P-graph or process graph framework is an extremely useful methodology as a modeling tool in various areas. P-graphs are directed bi-partite graphs that give an unambiguous representation of any process that can be expressed as a network. It is based on rigorous axioms and combinatorial analysis. Here we apply the methodology to the design of supply chains for sustainability. The result is a maximal structure, solution structures, and an optimal structure of the network for the process of interest. All of these are feasible and meet design requirements. There are freely available software (PNS Studio and PNS Draw) which automate much of the application of the methodology. The P-graph framework is most useful in the initial design phase of a process where the requirements, the feedstocks, the outputs, and the necessary process structure or network may not be precisely defined. But there is a need to generate alternatives which are feasible to start the design process. When coupled with sustainability considerations, it is possible to effectively generate design options that are cheaper and more sustainable than currently used designs. The method can be further applied to steady state and none-steady state operations. Examples illustrating the use of the methodology with sustainability considerations will be presented.

Thursday Plenary Session II

Thursday, March 12, 2015 (Ballroom)

1:00 PM **Plenary Introduction**

David Venerus (Illinois Institute of Technology)

1:10 PM **Collide and Conquer: Flow-induced Segregation Phenomena in Blood and Other Multicomponent Suspensions**

Michael Graham (Distinguished Professor, University of Wisconsin-Madison)

Blood is a suspension of particles of various shapes, sizes and mechanical properties and the distribution of these particles during blood flow is important in many contexts. Red blood cells (RBCs) tend to migrate toward the center of a blood vessel, leaving a so-called cell-free layer at the vessel wall, while white blood cells (WBCs) and platelets are preferentially found near the walls, a phenomenon called margination that is critical for the physiological responses of inflammation and hemostasis. Potential beneficial effects on hemodynamics arise from addition of high molecular weight long-chain polymer molecules known as drag-reducing additives (DRAs) to blood; one effect of these additives is the reduction of the cell-free-layer thickness. Additionally, the segregation properties of WBCs, platelets, and RBCs can be employed for their separation or detection in microfluidic devices. Finally, drug delivery particles in the bloodstream will also undergo segregation phenomena – the influence of these phenomena on the efficacy of such particles is unknown.

This talk describes efforts to gain a systematic understanding of flow-induced segregation phenomena in blood and other complex mixtures, using a combination of theory and direct simulations of flowing suspensions. Two specific issues are addressed here: (1) the origin of the margination phenomenon and its dependence on the relative properties of the different types of suspended particles in a mixture and (2) the effect of DRAs on the formation of the cell-free layer. The study of margination reveals that this phenomenon is strongly affected by the nature of pair collisions between different types of particles during flow. A kinetic theory model based on pair collisions and wall-induced hydrodynamic migration can capture the key effects observed in direct simulations. In the case of polymer additives, the experimentally observed thinning of the cell-free layer is reproduced in simulations and the mechanism underlying it is described. Having in hand an understanding of the mechanisms underlying these phenomena now allows more rational approaches to development of quantitative models of them and processes that exploit them. This knowledge will also lead to a better understanding of the consequences of these phenomena in physiology and medicine.

Thursday Dinner Keynote

Thursday, March 12, 2015 (Ballroom)

6:50 PM Local Section Announcements

Azita Ahmadzadeh (UOP/Honeywell)

7:00 PM Keynote Introduction

Dennis O'Brien (Jacobs Consultancy)

7:10 PM How My Career Led to AIChE

June Wispelwey (Executive Director, AIChE Global)

My career has taken many twists and turns, but when it began, I never thought that leading AIChE and its efficient growth would be my mantra. Upon reflection, the choices I made and the passion I have led me to the Institute. During this talk, I will discuss my career choices and how they relate to the AIChE of both today and tomorrow.

Friday Morning Keynote Session

Friday, March 13, 2015 (Ballroom)

8:00 AM Volunteer Recognition

Jerry Wilks (CITGO)

8:10 AM Keynote Introduction

Paolo Palmas (UOP/Honeywell)

8:20 AM Refining Technology and Configuration for Future Fuels

Chris Gosling (UOP/Honeywell)

Petroleum refining utilizes a wide range of separation, conversion, and treating technologies to convert crude oil of varying quality into today's clean gasoline and diesel fuels. The technical objectives of petroleum refining operations and the basic process units that are utilized to convert various petroleum fractions to fuel blending components will be discussed. In addition, how the individual refining process units are configured to meet local and export demands for fuel production, ranging from simple hydro-skimming to full conversion configurations will be reviewed.

Fuel production is becoming increasingly complex as modern Clean Fuels regulations are adopted worldwide. This has required the integration of new petroleum refining technology to economically maximize the production of Clean Fuels. Existing Clean Fuels regulations, potential future fuels, and what refining technology will be needed to produce these fuels will be discussed.

Friday Plenary Session I

Friday, March 13, 2015 (Armour Dining)

1:00 PM Plenary Introduction

Trey Morrison (Exponent)

1:10 PM Do We Really Need More Process Safety Leadership?

Peter Lodal (Technical Fellow, Eastman Chemical Company)

Process safety, as is the case with many other disciplines, emphasizes the need for strong leadership and commitment. Leadership from the top is a critical element in any process

safety program, but it is a necessary, not a sufficient condition for success. In this presentation, the need for competent followership will be discussed and illustrated.

Friday Plenary Session II

Friday, March 13, 2015 (Ballroom)

1:00 PM Plenary Introduction

Georgia Papavasiliou (Illinois Institute of Technology)

1:10 PM Systems Tissue Engineering

Lonnie D. Shea (Professor and Chair of Biomedical Engineering, University of Michigan)

Systems and strategies for promoting tissue growth provide enabling technologies for either enhancing regeneration for diseased or injured tissues, or to investigate abnormal tissue formation such as cancer. Given the complexity inherent in tissues, my laboratory is working towards the concept of "Systems Tissue Engineering", which indicates, in part, the need to develop systems capable of presenting combinations of factors that drive tissue growth. Biomaterial scaffolds represent a central component of many approaches and provide the enabling tools for creating an environment and/or deliver factors that can direct cellular processes toward tissue formation. The presentation will illustrate this approach through our work with islet transplantation in Type 1 Diabetes therapy. The scaffolds aim to create an environment that supports robust engraftment of transplanted islets through integration with the host tissue. Due to integration with the host tissue, we have also developed strategies for local immunomodulation, as well as the development of nanoparticles for antigen-specific tolerance to address both the autoimmune disease and allogeneic response to the transplanted cells.

Closing Keynote

Friday, March 13, 2015 (Ballroom)

4:30 PM Keynote Introduction

Martin R Gonzalez (BP)

4:40 PM The Shale Gas revolution in the US

Henrik Rasmussen (Vice President of Catalyst and Technology, Haldor Topsoe)

The presentation will describe the consequences for the petrochemical industry and the refining business and the shift in strategy for both industries. Will discuss the opportunities for new technology such as GTL in the US due to shale gas and tie in the EPA regulation on NOx and Sulfur to maintain a clean environment while expanding the industry. In closing I will comment on the job opportunities for chemical engineers in today's environment.

AIChE Midwest Regional Conference

Presentation Abstracts

Refinery Integrity Management

Thursday, March 12, 2015 (Ballroom, ThA1)

Chair: *Jerry Wilks* (CITGO Petroleum)

9:30 AM (ThA1a) High Temperature Damage Mechanism in Refinery Environments

Bernard Schulze (Stress Engineering Services)

High temperature hydrogen attack (HTHA) and creep are common damage mechanisms found in refinery applications. Both mechanisms are challenging to identify and detect during the incipient states of damage. An overview of materials and operating conditions that are susceptible to these mechanisms will be discussed. A review of damage modeling and damage tolerance will be provided. Inspection types and detection limits will be discussed as part of an overall equipment integrity strategy.

9:55 AM (ThA1b) CFD Investigation of a Hydrogen Reformer Furnace for Improved Flow Distribution

Bin Wu, Chenn Q. Zhou, Armin Silaen (Purdue University Calumet)

A hydrogen reformer furnace is a combustion chamber used to supply heat for the catalytic process that converts natural gas into hydrogen. The reforming reaction that happens inside the catalyst tubes is endothermic and requiring high levels of heat input. The combustion process in the hydrogen reformer furnace provides the heat to maintain the chemical reaction inside the tubes. Consequently, heat control in the hydrogen reformer furnace is one of the most important factors for the catalytic reforming process. The previous investigation indicates the uneven heat distribution inside the furnace has caused the aging issue of catalyst tubes. Hence, optimization of heat distribution inside the furnace is a vital step of the catalytic reforming process. Utilizing the multiphase and non-premixed model of CFD (Computational Fluid Dynamic), the thermal behavior inside the furnace has been investigated. Results revealed that both the gaps on the sidewall of the tunnel and the location of air distribution wall have impact on the temperature distribution of catalyst tubes. The performance of each configuration with different parameters is carried out to provide a great deal of insight for industry field.

10:20 AM (ThA1c) Analysis of Refinery Equipment to Improve Unit Start-ups and Shut-Downs

Jerry Wilks (CITGO Petroleum)

In the Oil Industry much of the equipment operates at high enough temperatures to avoid the risk of brittle fracture during typical operations. However, there are start-up and shut down periods that subject pressure vessels and piping to combinations of stress and low temperature that could lead to

brittle fracture. In the past, the risk of equipment failure led to the development of start-up and shut-down procedures that sometimes require long delays. To minimize the time required for unit start-up and shut down, brittle fracture analysis of refinery equipment is being conducted today to determine the acceptable operating temperatures over the range of pressures. The guidelines in API 579 are usually used for these analyses. The results of these analyses are the generation of graphs called "safe pressurization curves". Operations that keep the operating conditions above these curves can be used to shorten start-up and shut-down time periods thereby saving refineries money. There is also a risk of brittle fracture during auto-refrigeration events associated with pressure changes in light hydrocarbon systems, and brittle fracture analyses can also deal with auto refrigeration risks. This paper provides background information on brittle fracture analysis along with several examples of brittle fracture analysis of refinery equipment. Examples that show the effects of past process conditions on the results of brittle fracture analysis are also reviewed.

10:45 AM (ThA1d) Application of Metal Oxides to Alleviate Corrosion from Chlorides

Hans-Christoph Schwarzer, Axel Düker (Clariant)

Corrosion in refineries is a serious problem and is often related to chlorides, which cause pitting corrosion, as well as stress corrosion cracking, depending on applied materials and conditions. Chlorides in refineries may occur in different streams. A typical location for chloride-caused corrosion issues is downstream of the catalytic reformer unit. All chlorides that are fed into that unit will be found in the product streams. For this reason most refineries have installed chloride guard reactors to capture the chlorides.

Many operators aim for HCl removal only when specifying their chloride guard performance. This approach may appear beneficial at first glance as it allows the use of promoted alumina guards. The drawback, however, is that organic chlorides are not captured. Thus, one of the main purposes of the Cl-guard installation is not achieved. Furthermore, alumina-containing guard materials develop catalytic properties similar to the catalytic reformer catalyst as their surface gets chlorinated. As a result, instead of removing HCl, alumina-containing Cl-guards convert HCl into organic chlorides. If only HCl concentrations downstream of the Cl-guard are monitored, it is only a matter of time until there is undetected chloride breakthrough.

To prevent this and to fully capture all Chlorides, high-tech Cl-guard materials have to be used. Such materials do not contain alumina or other materials that easily develop undesired properties when chlorinated. A very suitable guard material is

zinc oxide which provides high HCl pick-up capacities. Combined with the right binders and promoters, it can be engineered into a full-spectrum chloride guard that not only removes HCl, but also organic chlorides at high pick-up capacities. In addition, neither the formation of organic chlorides or green oil is observed, thus providing the best available protection against corrosion.

Advances in Bioremediation of Chemical Contaminants

Thursday, March 12, 2015 (Armour Dinning, **ThA2**)

Chair: Jarad L. Champion (Geosyntec),

Co-chair: Pahola Thathiana Benavides (VRI-Custom)

9:30 AM (ThA2a) Advances in 1,2,3-TCP Remediation in Groundwater via Biological Reduction

Melissa Schmitt, Eric Suchomel, Sandra Dworatzek, Jeff Roberts, Phil Dennis (Geosyntec Consultants)

1,2,3-trichloropropane (TCP) was used historically as a paint and varnish remover, a cleaning and degreasing agent, a cleaning and manufacturing solvent, and was a common component of soil fumigants previously used widely in agriculture. TCP is characteristically mobile in the subsurface and resistant to natural attenuation, and its persistence has resulted in wide-spread impacts on water supply systems. The U.S. Environmental Protection Agency (EPA) is evaluating TCP as part of the Third Unregulated Contaminant Monitoring Rule (UCMR3), which is used to determine whether a contaminant will be subject to future regulation, while individual states have or are in the process of developing goals for TCP that are as low as 0.0005 micrograms per liter.

Geosyntec has been a practice leader in the development and application of in situ bioremediation (ISBR) for TCP. TCP has been successfully remediated with bioremediation techniques, but with limited understanding of the degradation pathways and mechanisms for degradation and limited ability to detect potential degradation daughter products or secondary indicators of biodegradation such as relevant microbial populations. As such, Geosyntec has recently conducted TCP research to understand the extent to which Dehalogenimonas, a bacterium capable of TCP reduction, is naturally present in groundwater at sites with TCP; whether SiREM's KB-1[®] Plus bioaugmentation, which contains Dehalogenimonas, can be successfully used to enhance biodegradation of TCP in groundwater; and if so, what are the practical limitations of TCP bioremediation.

Under this research effort, Geosyntec used opportunities at two confidential Sites to study TCP bioremediation further. At Site #1, ISBR was previously implemented from 2000 to 2009 via injection of a soluble electron donor. While this ISBR program was successful, it is not clear whether TCP was degraded through biologically-catalyzed reduction or through abiotic chemical reduction, and the potential for ISBR of TCP at lower concentrations typical of many TCP plumes could not be determined. The presence of Dehalogenimonas in groundwater from the former source area has recently been evaluated to

see if reductive dechlorination by Dehalogenimonas is the probable mechanism for TCP degradation in this area of the site.

At Site #2, the overseeing regulatory agency has requested that a remedy be implemented to address TCP and 1,2-dichloropropane (DCP, a common co-contaminant with TCP) in groundwater at and downgradient of the Site. A treatability study has been conducted to evaluate ISBR options for Site, where the two electron donors and bioaugmentation using KB-1[®] Plus were evaluated. During the treatability study, the following were evaluated: the lower practical concentration limit for TCP that can be biologically reduced at relevant rates for ISBR and/or monitored natural attenuation, pH ranges over which degradation occurs, the intermediary degradation products, and the co-relation of Dehalogenimonas populations with the presence/concentration of TCP and possible breakdown products at the Site and in the microcosms (particularly at TCP and DCP concentrations). Based on the results, Geosyntec and SiREM have enhanced the understanding of TCP degradation via biological reduction, supporting ISBR as an effective means for TCP reduction in groundwater.

9:55 AM (ThA2b) Using Correlations to find Causations: a Statistical Model to Direct PCB Bioremediation Studies

Amanda Hughes (Geosyntec Consultants) *Mitch Small, Jeanne VanBriesen* (Carnegie Mellon University)

Biodegradation of polychlorinated biphenyls (PCBs) via dechlorination can significantly contribute to monitored natural recovery (MNR) in sediment. Accurate identification of dechlorination is critical because it alters the masses of congeners, and human health risk is congener-specific. The dechlorination of 209 PCB congeners can occur via 840 possible dechlorination pathways, which describe the loss of a chlorine atom from a higher-chlorinated congener to a lesser-chlorinated congener or biphenyl. Correct identification of dechlorination pathways by specific microorganisms will inform congener-specific bioremediation efforts.

Currently, pathway occurrence is extrapolated from observed changes in select congener masses within sediments over time. Such extrapolations have necessarily relied on the knowledge and experience of the researcher and therefore may neither be accurate nor reproducible. To address these concerns, a Bayes Monte Carlo (BMC) dechlorination pattern estimator (DPE) was developed to predict the likelihoods of eight previously identified dechlorination patterns.

The statistical approach presented here estimates the occurrence of eight previously identified dechlorination patterns using initial and final distributions of the 209 PCB congeners and biphenyl as input. It applies the BMC method such that 10,000 simulations are weighted according to the normal likelihood function. The DPE has four distinct advantages over the previous approaches. First, expert opinion is quantified in Bayesian prior distributions, which are subsequently updated with data. Second, the initial congener

distribution is not limited to an Aroclor. Third, dechlorination pathways in occurring patterns are not all assumed to be occurring. Finally, all dechlorination pathways and all congeners are simulated. Eighteen synthetically dechlorinated congener distributions are evaluated by the DPE to validate this approach.

The DPE was successfully validated and used to evaluate the occurrence of dechlorination patterns in a laboratory study of sediment from the Grasse River (NY, USA). This statistical approach indicated that a yet to be identified dechlorination pattern, which shares some of the same pathways with the identified patterns, is occurring in the Grasse River. In addition to identifying new dechlorination patterns, application of the DPE can be used to understand the complex relationship between biogeochemical parameters, microbial activity and the occurrence of specific dechlorination pathways, which can ultimately inform bioremediation of PCB-contaminated sediment.

10:20 AM (ThA2c) **Bioremediation at Low pH - Emerging Tools and Approaches for Chlorinated Solvent Sites**

Phil Dennis, Sandra Dwaratzek, Jeff Roberts, Peter Dollar (SiREM)

Bioremediation of chlorinated ethenes and many other chlorinated compounds is optimal at neutral pH with pH's below 6.0 considered problematic for bioremediation. For example, complete biodegradation of chloroethenes to ethene, is often inhibited below pH 6.0. Given that both reductive dechlorination and fermentation of commonly used electron donors are acid generating processes, enhanced bioremediation has the potential to decrease pH into the inhibitory range, even if prior to biostimulation, pH was acceptable.

In recent years, modifying aquifer pH using buffering agents such as sodium bicarbonate and various commercial formulations has become increasingly common. Aquifer pH modification has met with varying degrees of success depending on application method, site geology and geochemistry but is generally considered challenging. Effective alternatives or complimentary approaches would be welcome and could improve bioremediation outcomes.

In certain cases, especially where pH is near or slightly below 6.0, the use of bioaugmentation cultures acclimated to lower pH has the potential to reduce the need for aquifer neutralization. Increasing evidence indicates that complete dechlorination to ethene is possible below pH 6.0 with pH tolerant bioaugmentation cultures. Also, previous studies have indicated that certain electron donors have a reduced acidification impact, particularly formate (McCarty et al., 2007) which generates neutralizing bicarbonate alkalinity upon fermentation. The use of electron donors with reduced pH impact, combined with pH tolerant bioaugmentation cultures has the potential to achieve successful bioremediation results with reduced need for aquifer pH adjustment.

The development and field use of low pH acclimated cultures will be discussed and case studies presented. At a Site in Florida, with the pH ranging between 5.5 and 6.0, PCE, TCE and cDCE were completely dechlorinated to VC and ethene within 6 months of bioaugmentation with a low pH tolerant bioaugmentation culture.

10:45 AM (ThA2d) **In-situ Bioremediation and ZVI Injections for Source Abatement, Beneath an Active Manufacturing Facility**

Chriso Petropoulou, Valerie Bosscher, J. Neil Couch, Sean Carbonaro, Mary DeFlaun (Geosyntec Consultants), Jeff Roberts (SiREM)

Historic operations at an active manufacturing facility have resulted in light non-aqueous phase liquid (LNAPL), containing petroleum hydrocarbons and chlorinated solvents, in shallow source areas beneath the facility floor. In 2010, in-situ source abatement of the LNAPL smear zone was conducted by injection of micro-scale zero valent iron (ZVI), Newman Zone[®] Emulsified Vegetable Oil (EVO), and a consortium of dehalogenating bacteria (SiREM KB-1[®] Plus). Three years of post-injection monitoring indicate reducing, near-neutral conditions, relatively high concentrations of dehalogenating bacteria and available electron donor, diminished concentrations of parent compounds, and significant production of dissolved ethane and ethene. Supplemental injections were designed based on the conceptual site model, bench-scale treatability testing, and groundwater modeling, to proactively address elevated levels of intermediate degradation by-products such as 1,1-dichloroethane; cis-1,2-dichloroethene; and vinyl chloride in a targeted portion of the source area, which had limited electron donor and microorganism concentrations, resulting in slower degradation rates for the contaminants of concern. The supplemental injections of EVO, potassium bicarbonate buffer, and SiREM KB-1[®] Plus were implemented in December 2013. Post-injection groundwater monitoring conducted in 2014 indicates the supplemental source area amendments have enhanced the reductive dechlorination of intermediate degradation by-products, including vinyl chloride, in the targeted source area.

Advances in Pharmaceuticals

Thursday, March 12, 2015 (Alumni Lounge, **ThA3**)
Chair: *Zoltan K. Nagy* (Purdue University)

9:30 AM (ThA3a) **Decoupling of Spherical Crystallization Mechanisms in a Two-Stage MSMMPR**

Ramon Peña, Zoltan K. Nagy (Purdue University)

Of utmost importance in the crystallization of active pharmaceutical ingredients (API) in the pharmaceutical industry is to produce crystals of good physical, processing, and pharmacological properties. The definition of good physical properties depends on what the end goal and the drug formulation that the crystals will be a part of, but often times processing and pharmacological properties are competing

interests. Herein a concept and method to help satisfy both processing and pharmacological interests is proposed. The concept is to decouple the nucleation, growth, and agglomeration mechanisms. Decoupling will offer more degrees of freedom for the control of each mechanisms. This in turn provides the means by which properties in the nucleation/growth stage can be tailored to those of most pharmacological benefit and efficacy (e.g. bioavailability, dissolution, morphology) while allowing the agglomeration stage to be tailored to produce spherical agglomerates of the most processing efficiency (e.g. filtering, drying). Figure 1 depicts a schematic representation of the experimental setup for the continuous MSMPR.

The contribution of the work presented herein is spherical crystallization in a continuous two-stage mixed suspension, mixed product removal (MSMPR) crystallizer. The purpose of the proposed two-stage MSMPR crystallizer setup is to decouple nucleation/growth and agglomeration mechanisms. The continuous production of spherical agglomerates allows for changes in operating parameters to produce agglomerates of different qualities.

9:50 AM (ThA3b) **Combined Product and Process Design of a Multi-Stage Mixed-Suspension-Mixed-Product Removal (MSMPR) Cooling Crystallization System under Dissolution, Growth and Nucleation Mechanisms**

David Acevedo, Zoltan K. Nagy (Purdue University)

This work demonstrates the effect of considering dissolution, growth and nucleation on the crystals produced and design of a MSMPR cascade system and. The first step was to evaluate two MSMPR cascade configurations were evaluated: nucleation-growth (NG) and nucleation-dissolution-growth (NDG) using paracetamol as model system. Simulation results demonstrate that adding a dissolution step has an impact on the final crystal properties. Larger crystals and narrow distribution were obtained due to the removal of fine crystals through the continuous process experimentally. The second part of the study was to determine the optimal configurations that would maximize the mean size of the final crystal considering the various mechanism. The population balance model (PBM) was solved using a high resolution finite volume method considering primary and secondary nucleation, growth and dissolution kinetics. The optimal temperature and residence time of each stage was obtained and demonstrates that the optimal configuration is the NDG MSMPR system evaluated previously. The formulation was extended up to a MSMPR cascade system with five stages. The proposed configurations demonstrate high potential for improving the crystal size and distribution due to fines removal by considering dissolution, growth and nucleation mechanisms in the model formulation.

10:10 AM (ThA3c) **Advanced Control Approaches for Combined Cooling/Antisolvent Crystallization in Continuous Mixed Suspension Mixed Product Removal Cascade Crystallizers**

Yang Yang, Zoltan K. Nagy (Purdue University)

In fine chemical and pharmaceutical industry, the control of crystallization process is essential in order to achieve crystals with desired size distribution, shape and polymorphic form. Because these crystal properties can have large influence on the efficiency of downstream operations (e.g. filtration, drying, milling), as well as the physical and chemical properties (e.g. bioavailability, dissolution rate) of the final active pharmaceutical ingredient (API). Although batch crystallization is commonly used due to great operating flexibility and short development time, in principle continuous crystallization can have much better product quality consistency, process and equipment efficiency, and productivity. This study is the first one that investigates advanced control architectures for continuous crystallization systems. In a continuous two stage mixed suspension mixed product removal (MSMPR) crystallizer, the crystal size and yield are controlled simultaneously by manipulating temperatures and antisolvent addition rates at both the first and the second stages. A four by two multi-input multi-output (MIMO) control system is studied in detail. Not only nucleation and growth, but also dissolution kinetics are considered in this work. Based on various selections of manipulated variables, five control approaches (nucleation control, growth control, antisolvent control, temperature control and global control) are discussed and compared. The attainable regions of crystal size and yield using the proposed five methods are obtained. In addition, the feasibility of two advanced control approaches, decentralized proportional-integral-derivative (PID) control and nonlinear model predictive control (NMPC) is analyzed. Decentralized PID control is proved infeasible based on local linearization method and relative gain array (RGA) analysis, indicating that this process requires more advanced control approaches, such as NMPC, for smooth operation. It is found that the necessary and sufficient condition for NMPC to be feasible is that the set-point must be within the corresponding attainable region of that particular control method. In general when this condition is met, NMPC scheme shows good control performance for fast target product quality (size) and process requirement (yield) change-over, as well as process disturbances rejection. It is also shown that the non-square global control approach with four manipulated inputs (temperatures and antisolvent addition rates in both stages) provides faster closed-loop response and the largest attainable region.

10:30 AM (ThA3d) **Closed-Loop Control for the Feeder and Blender Unit Operations into the Continuous-Tablet Manufacturing Process**

Mariana Moreno, Zoltan K. Nagy, Gintaras V. Reklaitis, Arun Giridhar (Purdue University)

The pharmaceutical industry has traditionally operated with batch manufacturing with manual process control. Product quality is ensured by after-the-fact sampling and rejection of batches that fail quality assurance tests. As the adoption of continuous manufacturing and closed-loop control in the field

are currently increasing, adapting classical control techniques like PID and Model Predictive Control (MPC) for pharmaceutical systems become important to ensure product quality. Such activities have already been carried out for unit operations like the roller compactor[1].

In this project, we examine continuous powder blending, consisting of a feeder-blender subsystem, an operation that is used widely in multiple manufacturing processes for multiple product forms. It is desired to control the flow rate and composition of blended powder, and to ensure its blend uniformity, by manipulating the mass flows of individual components being blended together and the blender operational parameters. We present a comparison of multiloop PID control, linear MPC and nonlinear MPC, and how they perform for continuous blending. Finally, this work is compared to previous models presented in the literature.

[1] Hsu, S.; Reklaitis, G.V.; Venkatasubramanian, V. Modeling and Control of Roller Compaction for Pharmaceutical Manufacturing. Part II: Control System Design. *J. Pharm. Innov.* 2010, 5, 34-36.

10:50 AM (ThA3e) **Engineered Biosensor Proteins for Remote Control of Engineered Cell-Based Therapies**

Kelly Schwarz, Nichole Daringer, Rachel Dudek, Joshua Leonard (Northwestern University)

Engineered cell-based devices show great promise for clinical applications, such as harnessing the immune system to treat cancer. Controlling or modulating the functions of cell-based therapies post-implantation remains both attractive and challenging. For this purpose, my lab has developed a synthetic, self-contained, modular receptor system for mammalian cells for exclusive detection of extracellular cells such as proteins and cytokines. Here, I report the development of this technology to allow for the sensing and processing of physiologically relevant, endogenous cues using scFv-based antibody fragments for extracellular sensing and dCas9-VP64 for intracellular gene activation. This work establishes a technological foundation for using engineered receptors to control gene expression for applications spanning therapeutics, tissue engineering, and basic scientific research.

11:10 AM (ThA3f) **Development and Control of a Drop-on-Demand Manufacturing System for the Production of Melt-based Pharmaceuticals**

Elcin Icten, Arun Giridhar, Zoltan K. Nagy, Gintaras Reklaitis (Purdue University)

In recent years, the FDA has encouraged pharmaceutical companies to place renewed emphasis on the development of more innovative, efficient manufacturing methods with the use of process analytical technologies and the QbD approach. As part of this renewed emphasis on improvement of manufacturing, the pharmaceutical industry has also begun the selective transition from traditional batch processing to continuous manufacturing [1]. As a part of the NSF Engineering Research Center for Structured Organic Particulate Systems, a

mini-manufacturing process for drug formation has been developed. The process utilizes the drop-on-demand (DoD) printing technology for predictable and highly controllable deposition of active pharmaceutical ingredients (API) onto an edible substrate, such as a polymeric film or placebo tablet, using a semi-continuous operation suitable for flexible production of personalized dosage forms [2].

In this paper, we present a process narrative of the prototype system and discuss automation and supervisory control of the DoD manufacturing system along with the analysis of the drug forms created which consist of polymer and drug constituents. Implementing a supervisory control system for the manufacturing process, including automation and closed-loop control, is essential for producing individual dosage forms with precise control of dosage amount, morphology and formulation composition. The system consists of a positive displacement pump, xy-staging, imaging system and temperature controllers. The drop volume is monitored using the imaging system, to ensure consistent drop size and thus dosage amount. The xy-staging allows creating precise drop positioning while printing. Using this process, different drug formulations including solvent-polymer-API and polymer-API systems, i.e. co-melt systems, have been produced. Polymers are added to the printing material to help control drug morphology, material properties and the formulation composition [3]. Multiple temperature controllers are used to control the temperature of the process elements including material reservoir, pump, tubing and nozzle. Temperature control on the process allows maintaining printable rheological and material properties for the production of melt-based dosage forms. Temperature control on the substrate is crucial, since crystallization temperature has an effect on product quality, influencing the bioavailability of the drug [4]. After drop deposition, changes in drug morphology can be monitored using a spectroscopic technique, such as Raman, and corrected by temperature control action on the substrate. Using the proposed temperature control strategy on the substrate, the crystallization behavior is tailored to compensate for these variations and achieve consistent drug morphology.

[1]. K. V. Gernaey, A. E. Cervera-Padrell, and J. M. Woodley, "A perspective on PSE in pharmaceutical process development and innovation," *Computers & Chemical Engineering*, vol. 42, pp. 15–29, Jul. 2012.

[2]. L. Hirshfield, A. Giridhar, L. S. Taylor, M. T. Harris, G. V. Reklaitis, "Dropwise Additive Manufacturing of Pharmaceutical Products for Solvent-based Dosage Forms," *Journal of Pharmaceutical Sciences*, vol. 103, issue 2, pages 496-506, February 2014.

[3]. N. S. Trasi and L. S. Taylor, "Effect of Additives on Crystal Growth and Nucleation of Amorphous Flutamide," *Crystal Growth & Design*, vol. 12, no. 6, pp. 3221–3230, Jun. 2012.

[4]. E. Icten, Z. K. Nagy, G.V. Reklaitis, "Supervisory Control of a Drop-on-Demand Mini-manufacturing System for the Production of Pharmaceuticals," *Proc. of 24th Eur. Symp. Comput. Aided Process Eng. ESCAPE 24*, vol. 24, June 2014.

Renewable Energy Sources and Systems

Thursday, March 12, 2015 (Herman Lounge, **ThA4**)

Chair: *Jordan Ciezobka* (Gas Technology Institute)

9:30 AM (ThA4a) Gas Fermentation of Carbon Residues to Fuels and Chemicals

Rachel Brenc (LanzaTech)

Increasing worldwide demand for biofuels from renewable feedstocks is driving the rapid development of processes to produce low-carbon fuels and chemicals with lower greenhouse gas emissions compared to conventional petroleum derived products. LanzaTech's novel gas fermentation technology can economically convert gas containing carbon monoxide and any amount of hydrogen to fuel and chemical products. Initially developed to process industrial residue gas streams such as waste gases from steel mills, refineries, or petrochemical plants, the robust fermentation process can also utilize on-purpose syngas from the gasification of biomass, municipal solid waste, refinery residues (such as petcoke, vacuum residues, and heavy oils) and coal. The LanzaTech process can convert these gas streams into energy rich fuels or chemicals such as ethanol, acetic acid, or 2,3-butanediol, among others. A key differentiator of this biotechnology offering is the ability to produce a wide product slate from the same feedstock by utilizing different families of biocatalysts.

The LanzaTech's integrated thermochemical/biochemical gas fermentation process is described, highlighting the role of carbon recycling (capture and reuse) in the production of low carbon fuels and chemicals and demonstrating how low emissions (relative to fossil-derived products) can be achieved on various feedstocks. The process scale-up path from lab to pilot to pre-commercial demonstration will also be described, highlighting the feedstock flexibility of the process and technology integration at established industrial sites, as LanzaTech has now demonstrated at-scale the performance of its technology on a range of different gas inputs. Various pilot and demonstration activities will be described, including scale-up challenges faced to date, lessons learned from operating across varied global regions, and key activities that will lead up to LanzaTech's first commercial facility.

9:50 AM (ThA4b) Techno-Economic Analyses and Life Cycle Assessment of Two Stage Fast Pyrolysis for Bio-oil Production from Pine Wood

Olumide Winjobi, David Shonnard, Wen Zhou, Ezra Bar Ziv
(Michigan Technological University)

Thermochemical conversion of wood to biofuel via fast pyrolysis is regarded as a promising alternative for producing biofuels. This process involves a quick thermal degradation of wood in the absence of air at a temperature of approximately 530°C with a short residence time of less than 1 second in the pyrolysis unit. Despite its potential, one of the major drawbacks of this approach for production of biofuels is the process

energy intensity. Drying and size reduction of wood are major contributors to energy consumption and the development of a two stage process that involves a torrefaction pretreatment step prior to pyrolysis was investigated as an approach to minimize the energy consumption associated with the size reduction step. Torrefaction, often referred to as mild pyrolysis, tends to enhance bio-oil properties by reducing water content, minimizing acidity, and increasing heating value. The impact different torrefaction temperatures has on the cost of production as well as the environment has been investigated by carrying out techno-economic analysis (TEA) and environmental life cycle assessment (LCA) respectively, and the two stage processes will be compared to the one stage pyrolysis. However, the work reported here investigated a 2-stage process for producing pyrolysis oil. Benefits of heat integration will also be investigated for this work.

Aspen Plus process simulation package is used to model the two stage torrefaction-fast pyrolysis process. The effect of torrefaction severity on composition and yield of pyrolysis bio-oil was included using data from the works of Westerhof et al (2012)[3], Zheng et al (2012)[4], and Jones et al (2009)[1] while the work of Phanphanich et al (2011) [2] was used for the effect of torrefaction on size reduction energy requirements. Using these data, mass and energy balances are obtained, and then subsequently used in sizing the equipment, with equipment prices estimated from a number of sources such as the Aspen Economic Process Analyzer, previous works and equipment vendors. A Discounted Cash Flow Rate of Return spreadsheet prepared will be used to obtain the gate cost of production, and data obtained from the simulation will also serve as inputs for the LCA that will be carried out using the LCA software SimaPro 8.0.

From our model simulations, having a torrefaction step as a pretreatment step prior to fast pyrolysis reduces the cost of bio-oil production by reducing energy cost associated with size reduction. Results from the model also shows a reduction in GHG emissions associated with the bio-oil production system as a result of the torrefaction pretreatment step.

[1]. Susanne B Jones, Corinne Valkenburg, Christie W Walton, Douglas C Elliott, Johnathan E Holladay, Don J Stevens, Christopher Kinchin, and Stefan Czernik, Production of Gasoline and Diesel from Biomass Via Fast Pyrolysis, Hydrotreating and Hydrocracking: A Design Case Pacific Northwest National Laboratory Richland, WA, 2009).

[2]. Manunya Phanphanich, and Sudhagar Mani, 'Impact of Torrefaction on the Grindability and Fuel Characteristics of Forest Biomass', Bioresource technology, 102 (2011), 1246-53.

[3]. Roel J. M. Westerhof, D. Wim F. Brilman, Manuel Garcia-Perez, Zhouhong Wang, Stijn R. G. Oudenhoven, and Sascha R. A. Kersten, 'Stepwise Fast Pyrolysis of Pine Wood', Energy & Fuels, 26 (2012), 7263-73.

[4]. Anqing Zheng, Zengli Zhao, Sheng Chang, Zhen Huang, Fang He, and Haibin Li, 'Effect of Torrefaction Temperature on Product Distribution from Two-Stage Pyrolysis of Biomass', Energy & Fuels, 26 (2012), 2968-74.

10:10 AM (ThA4c) **Opportunities and Challenges for Energy-Intensive Chemicals: Emerging Technology Review**

Yuan Yao (Northwestern University), *Diane Graziano* (Argonne National Lab), *Matthew Riddell* (Argonne National Lab), *Eric Masanet* (Northwestern University)

Chemical industry is the largest energy consumer in the world, it accounts for 30% of global industrial energy use[1]. At the same time, chemical industry is one of major source of greenhouse gas emissions (GHG) that are mostly generated during fuel combustion in chemical process[2]. Growing energy demand and severe environmental problems is prompting the development of emerging technologies in chemical production process for energy consumption and adverse environmental impacts reduction. This presentation reviews emerging technologies for reducing fossil fuel inputs associated with production of ammonia, olefins (ethylene and propylene), BTX (benzene, toluene and xylenes), which are energy-intensive commodity chemicals (EICCs) according to IEA analysis, and their relatives. Available data of these technologies are harmonized to quantify the potential reduction of energy and GHG emissions, which can shed the light on where are opportunities.

This presentation includes two sections, the first part focuses on technologies still using fossil fuel. Currently, the production of EICCs mostly uses fossil fuel-based feedstock (e.g. natural gas and petroleum oil) and these chemical processes have been steadily improved over time[3]. Still, there are some novel technologies coming out from R&D efforts for better energy efficiency. The presentation will introduce and discuss the energy benefits, development stage, technology and cost barriers of a number of technologies relating to EICCs production. These technologies are either incremental technologies that can be retrofitted to improve the performance of current process (e.g., catalysis-assisted production of olefins) or new pathways using different fossil feedstocks (e.g., ethane oxidative dehydrogenation for ethylene production).

In the second section, technologies using alternative feedstock biomass and CO₂ to produce EICCs, their derivatives/substitute products are presented. Recent life cycle assessment (LCA) for these technologies are reviewed and will be presented for better understanding of their energy saving and GHG emissions mitigation. As high cost is one of the major concerns for alternative- feedstock-based technologies, economic data for these technologies compared with conventional production process are collected and presented to help audience to understand the risk factors and financial barriers.

The authors admit that this review is not comprehensive for all possible improvement due to large number and wide variety of novel technologies, instead, it focuses on technologies whose potential energy and GHG emissions reduction can be evaluated through recent and credible data from literature. These quantitative data provides a good reference for chemical manufactures, industry analysts and policy makers for better

understanding of technology options for production of EICCs and their relatives.

[1] IEA, "Chemical and Petrochemical Sector, Potential of Best Practice Technology and other Measures for Improving Energy Efficiency" IEA, France 2009.

[2] IPCC, "2006 IPCC Guidelines for National Greenhouse Gas Inventories" IPCC, Kanagawa, Japan 2006.

[3] IEA, ICCA, and DECHEMA, "Technology Roadmap, Energy and GHG Reductions in the Chemical Industry via Catalytic Processes" IEA, ICCA, DECHEMA, France 2013.

10:30 AM (ThA4d) **Advanced Electrocatalysts for Fuel Cells**

Vojislav Stamenkovic, *Dongguo Li*, *Yijin Kang*, *Dusan Strmcnik*, *Nenad Markovic* (Argonne National Lab)

Commercialization of polymer electrolyte membrane fuel cells requires from the current technology to provide long operational lifetimes at a minimized cost. These issues can be tied, to a large degree, to the sluggish kinetics of the cathodic oxygen reduction reaction (ORR) where significant quantities of precious metal based catalyst are required to produce optimal power. Ability to control structure at the atomic level can effectively tailor catalytic properties of materials, enabling enhancements in activity and durability. Intense research efforts are focused on development of efficient electrocatalysts with minimal amount of precious metal and low cost. Alloying Pt with non-noble metals was found to be effective approach in reducing the Pt content in electrocatalysts by increasing their intrinsic activity. It was demonstrated that the formation of a nano-segregated Pt(111)-Skin structure over a bulk single-crystal alloys could enhance the ORR activity (vs. Pt/C) by two orders of magnitude through altered electronic structure of Pt surface atoms [1-3]. In spite of large improvements, these materials cannot be part of electrochemical devices but their outstanding catalytic performance can serve to guide the research aimed to development of more active nanoscale materials that offer high surface area utilization. The effect of nanoparticle size, surface morphology, composition and near-surface composition, shape, architecture will be addressed. The main emphasis in this presentation will be on the caged, hollow nanoframes that offer a new direction in the catalyst development and great promise to meeting the performance goals [4]. The hollow interior greatly diminishes buried non-functional precious metal atoms, and their uncommon geometry provides a pathway for tailoring physical and chemical properties. The open structure of the Pt₃Ni nanoframes address some of the major design criteria for advanced nanoscale electrocatalysts, namely, high surface-to-volume ratio, 3D surface molecular accessibility, and optimal precious metal utilization. The approach presented here for the structural evolution of a bimetallic nanostructure from solid polyhedra to hollow highly crystalline nanoframes with controlled size, structure and composition can be readily applied to other multimetallic electrocatalysts.

[1] Stamenkovic et al. Science 315 (2007) 493.

[2] Stamenkovic et al. Nature Materials 6 (2007) 241.

[3] Wang et al. Nano Letters 11 (2011)919.

[4] Chen et al. Science 343 (2014) 1339.

10:50 AM (ThA4e) **Optimal Closed-loop Design of Grid Scale Energy Storage Systems**

Oluwasanmi Adeodu, Donald Chmielewski (Illinois Institute of Technology)

It is widely recognized that a major concern with renewable energy is the fact that wind and solar sources are non-dispatchable. That is, the power produced from renewable sources is dependent on environmental conditions and is likely uncorrelated with the power demand from load centers. While fossil based sources are dispatchable and currently have the ability to respond to the full range of consumer loads, the additional range imposed by renewable sources is expected to exceed the dispatch capability of these fossil plants at the point of 20% renewable power. Thus, many have advocated the use of massive energy storage systems to provide the additional level of dispatch capability required to maintain grid solvency.

11:10 AM (ThA4f) **Efficient Solar Thermal Integrated Power and Chemical Production Cycles for Uninterrupted Power Supply**

Emre Gençer, Mohit Tawarmalani, Rakesh Agrawal (Purdue University)

Limited fossil fuel reserves and increasing greenhouse gas (GHG) emissions from fossil fuels make it necessary to develop alternative renewable energy sources to meet energy needs. Advancements in renewable power production are especially important since electric power is the largest consumer of primary energy resources with the highest growth rate among alternate energy use sectors, and is currently responsible for >40% of the global CO₂ emissions. Among the renewable energy sources, solar energy is prominent due to its abundance. Yet intermittencies and land availability constraints for solar energy collection are the grand challenges for solar thermal power generation and demand a high efficiency solar power generation cycle that synergistically integrates energy storage.

Here, we introduce new alternative processes that produce and store solar thermal power efficiently to enable for round-the-clock power supply. Solar power production processes are evaluated based on the process sun-to-electricity (STE) efficiency that refers to the fraction of incident solar energy that is directly recovered as the net electricity output. The second metric of interest is the overall sun-to-electricity (OSTE) efficiency. It is the net STE efficiency averaged over 24 hours, i.e. accounting for energy storage and delivery of the stored energy while solar energy is not available.

The novel solar thermal power cycle has a potential to generate electricity with STE efficiencies greater than 30% at low solar heat collection temperature. The cycle also promises STE efficiencies greater than 40% for the high solar heat collection temperatures.

For the cases with higher solar heat collection temperatures,

the solar water with reheat power cycle is modified by coproducing chemicals for storing energy from solar irradiation. When solar energy is not available, we propose the use of the same power cycle. This is achieved by addition of combustors that burn the stored chemicals to provide the high temperature heat. The overall sun-to-electricity efficiency of a twenty-four hour cycle is estimated to be greater than 30%. In summary, we propose a thermodynamic cycle that has the potential to generate uninterrupted electricity for grid distribution around the clock at GWh levels.

Fundamentals of Process Modeling and Equipment Design

Thursday, March 12, 2015 (Ballroom, ThB1)

Chair: *Rajeswar Gattupalli* (UOP/Honeywell)

Co-chair: *Adam Kanyuh* (UOP/Honeywell)

2:15 PM (ThB1a) **Molecular Dynamics Simulation of Gas Solubility in n-Alkanes and n-Alcohols**

Kevin R. Hinkle (UIC), *Paul M. Mathias* (Fluor), *Sohail Murad* (Illinois Institute of Technology)

We have improved the estimation of the solubility of hydrogen and carbon monoxide in a range of linear alcohols and alkanes (between C₄ and C₃₂) by using the method of molecular dynamics (MD) together with experimental data and traditional thermodynamics analysis. The goal of the study was to use a fundamental molecular-based method, after validation, to fill gaps in data in current literature, especially for systems considered challenging for traditional measurement and estimation methods. The simulation system used semi-permeable membranes to mimic actual experimental studies of gas solubility. Our combined analysis of both data and simulation results demonstrated that for higher carbon numbers (C_n) both CO and H₂ individually have similar Henry's constant values in the two solvents, with H₂ values being roughly 50% higher in both solvents. The data and simulation results were also used to estimate limiting values of the mass-based Henry's constant for H₂ and CO in the higher alcohols (large C_n).

2:35 PM (ThB1b) **Accuracy of Predictive Thermodynamic Models for Modeling Difficult Separation Processes**

Eric Cheuget (UOP/Honeywell)

Reliable process design and capital cost estimation of separation processes in refinery and other petrochemical processes requires accurate thermodynamic models for process simulation. In many cases phase equilibrium data for potential processes are not available and predictive thermodynamic models must be used to estimate the phase equilibria in the system. A popular traditional predictive model is the UNIFAC model which is based on empirical molecular group contributions. A newer approach is the COSMO model which is based on molecular surface properties derived from quantum chemistry. This study examines the accuracy of these models for modeling two types of mixtures: 1) hydrogen-

bonding phenolic-rich aqueous mixtures containing hydrocarbon and typical of the downstream processing of biofuels derived from pyrolysis oil; and 2) mixtures of polar solvents and close-boiling C4-C6 hydrocarbon alkane/olefin isomers typical of refinery process extractive distillation alkane/olefin isomer separations. The accuracy of the models is evaluated by comparing the predictions of the models with vapor- and liquid-liquid equilibria data available in the literature. The results indicate that, depending on the situation, these models may not yield predictions of sufficient accuracy for reliable process design.

2:55 PM (ThB1c) **Systematic Analysis and Convenient Prediction of Steady State Multiplicity Patterns**

Satish J. Parulekar (Illinois Institute of Technology)

Chemical and biological reactions with nonlinear kinetics when carried out in well-mixed reactors give rise to the possibility of reactor operation at multiple operating points at steady state. When multiple steady states are physically realizable, identification of various multiplicity regions in the space of reactor operating conditions is important for design, optimization and controlled operation of chemical and biological reactions. Prediction of steady state multiplicity patterns in terms of profiles of concentrations of species influencing reaction kinetics is important for better understanding of the reaction behavior and design, optimization and control of reactors used to conduct these reactions. These patterns are simpler with respect to certain operating variables, such as the feed concentration of a reactant, and complex with respect to other operating variables, such as the reactor space time. With reactor space time as the variable parameter, interesting patterns such as isolas and mushrooms have been reported for isothermal and non-isothermal reactor operation. In prior studies, these have been obtained via extensive iterations involving sweeps through parameter spaces. In this study, a convenient procedure for analyzing and predicting steady state multiplicity patterns is developed and illustrated considering one or more autocatalytic reactions as specific examples. Autocatalytic reactions and processes are commonly encountered in growth of all living cells, processes involving free radicals, polymerization processes, many inorganic and organic reactions, and crystallization processes. A comprehensive analysis of steady state multiplicity of single and two parallel/series autocatalytic reactions occurring in a well-mixed reactor is presented. The generation of the autocatalyst from competing or consecutive resources by cubic autocatalysis is followed by its decay. Parallel and series autocatalysis is observed in growth of living cells on multiple substitutable resources (nutrients) and co-metabolism of primary and secondary nutrients (simultaneous utilization of multiple nutrients via independent metabolic pathways inside living cells). A single well-mixed reactor may operate at up to three steady states for a single autocatalytic reaction and at up to five steady states for two parallel/series autocatalytic

reactions. Steady state multiplicity patterns are predicted in a non-iterative fashion by a judicious choice of parameter combinations. The space of ratios of the kinetic parameters for the autocatalytic reactions and ratios of supply of resources is divided into different regions depending on the maximum number of steady states admissible, which vary from three to five. The space of the remaining kinetic and operating parameters is divided into multiple regions based on the number and identity of physically realizable steady states. This division allows exact determination of appearance and disappearance of particular steady states. Continuation curves for limit point (LP) bifurcation are identified in the multi-dimensional kinetic and operating parameter space. While the LP continuation curves have a single disposition for a single autocatalytic reaction, there is a wide variety of dispositions of these for two autocatalytic reactions. Concentration profiles of species participating in the reactions are predicted conveniently using the LP continuation diagrams. These are simple when feed composition is varied and the same is the case when reactor space time is varied in the absence of autocatalyst decay. With autocatalyst subject to decay, exotic patterns such as single and multiple isolas and mushrooms of different varieties, are possible with reactor space time as the variable parameter. The LP continuation diagrams enable convenient and precise prediction of emergence and extinction of isolas and mushrooms. A reversible sweep in a parameter combination as reactor space time is varied leads to interesting patterns of isolas and mushrooms. Two or more consecutive reactions are therefore necessary for admission of isolas and mushrooms. The reaction systems with two autocatalytic reactions exhibit rich varieties of steady state patterns. Some of these will be presented as specific illustrations. The present approach enables a much easier identification of the multitude of rich steady state multiplicity patterns.

3:15 PM (ThB1d) **Computational Fluid Dynamics (CFD) for Process and Equipment Design and Development**

Quan Yuan, Reza Mostofi-Ashtiani, Hadjira Iddir
(UOP/Honeywell)

Computational Fluid Dynamics (CFD) is a powerful tool for the analysis and solution of fluid flows that may involve additional physics such as chemical reactions, heat and mass transfer commonly encountered in refining and petrochemical processes. With the advancement of computer speed and CFD software in the past several decades, it has become a practical predictive tool for modeling large-scale industrial processes and equipments with complex geometry, allowing scientists and engineers to perform “numerical experiments” during different stages of research, development and engineering design. For example, combustion and heat transfer in a direct-fired process heater can be simulated using a detailed CFD model including all the relevant length-scales ranging from burner details to the radiant-box size. CFD results from such a model can help make data-driven decisions on the heater design and operating conditions for better process

performance, improved energy efficiency and increased operating sustainability. CFD can also be used to quantify the process performance and equipment reliability in multiphase flow systems. For instance, it can be used to predict catalyst flow distribution in refining processes and help improve equipment design. As an example, uniform distribution of catalyst is a crucial aspect of a gas-solids process unit and CFD can be used effectively to quantify this important performance characteristic. Another example is flow distribution in slow moving or fixed beds, where CFD can help optimize the flow distribution to meet the design target. This paper gives a brief overview of CFD and presents a few selected examples to demonstrate how CFD is routinely used as a design tool to assist process and equipment design or assist in field operating troubleshooting efforts at Honeywell's UOP.

3:35 PM (ThB1e) **Small-Scale LNGP with Modular SMR Technology**

Trevor Smith (UOP/Honeywell)

In North America, there is a renewed push and demand for cleaner, cheaper, locally supplied fuels for transportation and high-horsepower applications. One technology solution that has seen sustained growth throughout the world is the use of LNG. Thanks to abundant new supplies of shale gas, a large price spread has developed between North American LNG vs. diesel fuel. Combined with the environmental and safety benefits of natural gas, an energy arbitrage opportunity has emerged that encourages fuel substitution in long haul heavy-duty trucking and other high-horsepower applications (oil field, rail, mining) and for off pipeline gas power plants. This presentation will discuss the market fundamentals driving conversions to LNG, the primary natural gas pre-treatment and liquefaction technologies, and the value of modular production facilities.

3:55 PM (ThB1f) **A New Slurry Bubble Column Reactor for Diesel Fuel**

Dimitri Gidaspow, Yuting He, Vishak Chandra (Illinois Institute of Technology)

The availability of gas from fracking makes it economical to produce liquid fuels using Fisher-Tropsch technology. A recent ACS symposium, "Ultraclean Transportation Fuels" edited by Olayinka. I. Ogunsola and Isaac K. Gamwo[1] and perspective "The Impact of Shale Gas in the Chemical Industry" by Jeffrey J. Siirola[2], gave excellent reviews of the subject. The National Renewable Energy Laboratory[3] provides estimates of costs needed to construct reactors for such synthesis. In an excellent review of various reactors Krishna and Sie[5], state that the adiabatic temperature for this reaction is 1600 K. The adiabatic temperature with the flow of the liquid will be of the order of 16 K, due to the high density of the liquid versus that of the gases.

The new and patentable idea (Gidaspow Aug 28, 2014) is to remove the liquid product through an overflow system. The required temperature rise is only about 6 °C. The closest process

in the literature to this is the U.S. Bureau of mines oil circulation process carried out in a 1-bbl/day reactor 20cm diameter of a bed height of 2.4m using 8-16 mesh catalyst particles. We are using an extension of our multiphase computational fluid dynamics program described in the 2009 book by Gidaspow and Jiradilok[6] to design such reactors. We have shown that it is best to use large catalyst particles, such as those in the US Bureau of Mines process, rather than the fine particles used in the Air Products methanol slurry bubble column reactor[4]. The large catalyst particles allow the use of high velocities of the synthesis gas without blowing out the catalyst from the reactor. This leads to the design of smaller synthesis reactors without the use of expensive cooling tubes.

- [1]. Olayinka I. Ogunsola, Isaac K. Gamwo, Ultraclean Transportation Fuels, ACS Symposium Series 959, American Chemical Society(2007).
- [2]. Jeffrey J. Siirola, The Impact of Shale Gas in the Chemical Industry, AIChE Journal, Vol.60, 810-819 (2014).
- [3]P. L. Spath and D. C. Dayton, preliminary screening- technical and economic assessment of synthesis gas to fuels and chemicals with emphasis on the potential for biomass-derived syngas, National Renewable Energy Laboratory, NREL/TP-510-34929, December, 2003.
- [4]. Yuanxiang Wu, Dimitri Gidaspow, Hydrodynamic simulation of methanol synthesis in gas-liquid slurry bubble column reactors, Chemical Engineering Science 55 (2000) 573-587.
- [5]. U.S Bureau of Mines, in R. Krishna, S.T. Sie, Design and scale-up of the Fischer-Tropsch bubble column slurry reactor, Fuel Processing Technology 64(2003)73-105.
- [6]. Dimitri Gidaspow, Veeraya Jiradilok. Computational Techniques: The Multiphase CFD Approach to Fluidization And Green Energy Technologies. Nova Science Publishers, 2009.

Water and Wastewater: Treatment and Management

Thursday, March 12, 2015 (Armour Dinning, **ThB2**)
Chair: *Urmila Diwekar (VRI-Custom)*

2:15 PM (ThB2a) **Mercury Removal from Industrial Aqueous Streams**

Sravan Pappu, Andrea Foster, Rachel Mansfield (Johnson Matthey)

This paper aims to review the current status of Hg removal in refineries and other industrial processes from produced water streams. Hg removal from water will potentially see increased scrutiny from regulatory agencies, however measuring / removing such content has not been effectively addressed for refineries and other industrial operators. Such requirements can cause significant impact to businesses not ready to approach Hg content with solutions that are fit for purpose. Topics that will be included are the regulatory requirements and other drivers for Hg removal in water and novel advances in Johnson Matthey's Hg removal capability from water streams. Focus will be given to recent advances in removal technology and how refineries and other industrial users can address challenges they may face with mercury removal.

2:35 PM (ThB2b) **Optimal Design of Adsorbents for NORM Removal from Produced Water in Natural Gas Fracking – Part I: Group Contribution Method for Adsorption**

Pahola Thathiana Benavides, Urmila Diwekar, Berhane Gebreslassie (VRI-Custom)

Natural gas has become an essential energy resource in the U.S. due to the increasing demand of energy, the high oil prices, and the need of foreign oil independency. The improvement in the drilling technology has allowed the rapid expansion in gas production, especially for unconventional gas such as shale gas. Shale gas is natural gas trapped within fine-grained sedimentary rocks called shale formations. Hydraulic fracturing is used to extract natural gas from these formations. Although natural gas is cleaner-burning than coal or oil, there is a lot of controversy due to the environmental impact related to the water consumption and treatment. Hydraulic fracturing generates significant volumes of wastewater that contain dissolved chemicals, high content of salts, and significant levels of natural occurring radioactive material (NORM). Hence, one of the biggest challenges of this industry is to develop techniques for the prevention, remediation, and appropriate disposal of NORM. The overall objective of this work is to develop and implement a novel computational tool for high-throughput screening and selection of new adsorbents for NORM removal. In the first part of this paper series, we study the adsorption theory for NORM removal and develop new group contribution methods (GCMs) to predict specific properties of adsorbents based on their thermodynamics. Then, in the second part of this paper we develop a computer-aided molecular design (CAMD) framework that generates potential adsorbent candidates according to the properties developed by the GCMs

2:55 PM (ThB2c) **Optimal Design of Adsorbents for NORM Removal from Produced Water in Natural Gas Fracking – Part 2: CAMD for Adsorption of Radium and Barium**

Pahola Thathiana Benavides, Urmila Diwekar, Berhane Gebreslassie (VRI-Custom)

This is second paper in series in which we use computer-aided molecular design (CAMD) methodology to obtain optimal adsorbents for adsorption of natural occurring radioactive material (NORM) in the produced water from fracking of natural gas. CAMD is posed as a mixed integer nonlinear programming problem. A new algorithm called efficient ant colony optimization (EACO) is used to solve this optimization problem which involves capacity of adsorption as an objective function and structural feasibility and process conditions derived from produced water composition as constraints. New adsorbents for removal of radium and barium together and individually are derived from this exercise. These adsorbents show far greater capacity to remove radium and barium from produced water than state of the art adsorbents found in literature.

3:15 PM (ThB2d) **Life Cycle Mass Flow Analysis of Water Demand, Produced Water Output and Solid Wastes Associated with Shale Gas Development Areas: A First Step in Estimating Impacts**

Tom Hays (Gas Technology Institute)

As shale gas emerges as one of the world's most abundant, affordable and clean-burning sources of energy, growth in the development and production of these resources will require sourcing of water that does not compete with community water supplies and an improved understanding of potential impacts arising from the management of produced water and solid wastes within shale development areas. The characteristics of shale gas waters in the Barnett and Marcellus Plays and the major flowsheets describing water management in the shale gas industry will be presented. Shale gas development requires multiple wells being drilled from one or two pads in a well field with hundreds of well fields constructed and completed within each development area. It becomes clear from simple month-by-month rollup computations that the annual generation and quality of water to be handled as well as annual output of solid waste (including drilling waste) becomes highly dynamic --- constantly increasing and decreasing each year. Within each year of the construction stage of the life cycle of a county-size development area (25 mi x 25 mi), billions of gallons of water must be found (sourced), hundreds of thousands of truckloads must transport water to wellheads for performing hydraulic fracturing of the shale as a necessary step for initiating gas production, tens of millions of barrels of brine (collected as flowback water and produced water) must be reused or disposed of in an environmentally acceptable manner, and hundreds of thousands of tons of drilling waste and sludge must be carefully managed. Since water and waste management represent substantial annual costs of shale gas development, the economical and environmentally-acceptable management of these streams is critical to the sustainable development of shale gas plays in the U.S., Europe, and throughout the world. GTI has developed a computer model that computes total mass flows of water and solid wastes streams on a year-by-year basis that are needed for life cycle assessments of environmental issues that can potentially arise from future shale development across defined geographic regions. This model will be described and examples of life cycle forecasts will be presented.

3:35 PM (ThB2e) **Optimization Application in Water Distribution Networks Using Embedded Hydraulic Models**

Arpan Seth, Carl D. Laird (Purdue University)

According to OECD's environmental outlook report[1], by year 2050, the global demand for water is expected to increase by 130% for domestic use, 140% for electricity use, and 400% for manufacturing use. Simultaneously, the fast growth of large urban centers is going to require significant expansion in the existing public water distribution networks. As these networks become larger and more complex, new techniques are necessary to help design and operate these networks, and

secure them against harmful contamination incidents. Optimization has been used in many of these applications that include design problems like valve placement to minimize water leakage, operation problems like pump scheduling to minimize energy cost, and security applications like optimal sensor placement for early contaminant detection, and contaminant source identification. The complexity of these optimization problems is directly related to their modeling requirements. For problems like sensor placement, where the decision variables (i.e. sensor locations) have no impact on the network model, simulations can be performed to precompute scenario data that can then be used in a Mixed-Integer Linear Programming (MILP) formulation. For problems like source inversion, the network hydraulics can be assumed as known inputs to build a water quality model. Since these types of problems involve manipulation of the water quality, they require an embedded water quality model into the formulation, resulting in an MILP or Nonlinear Programming (NLP) formulation. On the other hand, problems like optimal pump scheduling to minimize operational costs and valve placement to minimize water leakage require manipulation of water hydraulics. The water network hydraulic model comprises of nonlinear pressure drop relationships. Additionally, discrete variables are often necessary to model on-line decisions like pump schedules. Thus, the resulting optimization problems are NLPs or Mixed-Integer Nonlinear Programming (MINLP) problems. Even more challenging problems arise in incident response applications like opening of selected fire hydrants to optimally flush out contaminant from the network. These types of problems require manipulation of network hydraulics in order to improve water quality. Thus, embedding both the water hydraulic model and the water quality model becomes necessary, resulting in an NLP or an MINLP formulation.

Majority of techniques proposed in the literature for solving network hydraulics related problems (NLPs and MINLPs) are simulation-optimization based methods that use EPANET [2] as a black-box. In this work, we propose rigorous optimization techniques for these problems (e.g., optimal pump scheduling, optimum valve placement) where the hydraulic model is directly embedded into the formulation. For the problems where the resulting formulation is an MINLP, we implement a tailored algorithm in Pyomo[3], which is an open source modeling and optimization tool based on Python. In order to solve problems with realistic large-scale networks, we focus on exploring decomposition techniques and parallel codes for solving NLP and/or MILP subproblems that arise in our MINLP solution algorithm.

[1]. OECD (2012). OECD Environmental Outlook to 2050: The Consequences of Inaction. OECD Publishing, Paris.

[2]. Rossman, L. (2000). EPANET 2:Users Manual. Cincinnati, OH: U.S. Environmental Protection Agency.

[3]. Hart, W. E., Laird, C. D., Watson, J., and Woodruff, D. L. (2012). Pyomo - Optimization Modeling in Python. Springer.

Computational Methods in Biomedical Engineering

Thursday, March 12, 2015 (Alumni Lounge, **ThB3**)

Chair: *Ali Cinar* (Illinois Institute of Technology)

2:15 PM (ThB3a) Surface-Functionalized Nanoparticle Permeation Triggers Lipid Displacement and Ion and Water Leakage

Priyanka Oroskar, Sohail Murad, Cynthia Jameson
(University of Illinois at Chicago)

Functionalized nanoparticles (NPs) are considered suitable carriers for targeted drug delivery systems. However, the ion and water leakage induced by permeation of these nanoparticles is a challenge in these drug delivery methods due to cytotoxic effects of some ions. In this study, we have carried out a series of coarse-grained molecular dynamics simulations to investigate the effect of length of ligands on permeation of a nanoparticle across a protein free phospholipid bilayer membrane. Water and ion penetration as well as incidence of lipid flip-flop events and loss of lipid molecules from the membrane are explored in this study while varying the ion concentration gradient, pressure differential across the membrane, nanoparticle size, length of ligand, and nanoparticle permeation velocity. Some results from our studies include: (1) The number of water molecules in the interior of the membrane during ligand-coated nanoparticle (LCNP) permeation increases with nanoparticle size, ligand length, pressure differential, and permeation velocity but is not sensitive to the ion concentration gradient. (2) Some lipid molecules leave the membrane by being entangled with ligands of the NP instead of completing the flip-flop that permits them to rejoin the membrane thereby leading to fewer flip-flop events. (3) The formation of water chains or water 'fingers' provides a mechanism of ion transport across lipid bilayer membranes, but such ion penetration events become less likely for sodium ions than chloride ions and less likely for nanoparticles with longer-ligands.

2:30 PM (ThB3b) Stochastic Optimal Control for Prediction of Robust Drug Dosing Policies in Superovulation Stage of In-Vitro Fertilization

Kirti M. Yenkie, Urmila Diwekar (VRI-CUSTOM and UIC)

In-vitro Fertilization (IVF) is the most preferred technique for treatment of infertility among the methods of Assisted Reproductive Technologies (ART). It has been divided into four stages; (i) superovulation, (ii) egg retrieval, (iii) insemination/fertilization and (iv) embryo transfer. The first stage of superovulation is a drug induced method to enable multiple ovulation, i.e., multiple follicle growth to oocytes or matured follicles in a single menstrual cycle. IVF being a medical procedure that aims at manipulating the biological functions in the human body is subjected to inherent sources of uncertainty and variability. Also, the interplay of the hormones with the natural functioning of the ovaries to stimulate multiple ovulation in the first stage of superovulation as against a single ovulation in a normal menstrual cycle makes the procedure

dependent on several factors like the patient's condition in terms of cause of infertility, actual ovarian function, responsiveness to the medication. The treatment requires continuous monitoring and testing and this can give rise to errors in observations and reports. Thus, to predict the optimal hormonal dosing policies for enhanced superovulation, requires the incorporation of these measurement uncertainties for robust results. This work includes the measurement noise in the clinical data in the model development for follicular growth and number prediction, resulting in a set of stochastic differential equations (SDEs). This stochastic model in the form of SDEs is then used as the basis for predicting the robust drug dosing policies by application of stochastic optimal control methods.

2:45 PM (ThB3c) **Energy Expenditure Modeling and Its Use in Glucose Concentration Predictions**

Thiago Marques Luz Paulino, Ali Cinar, Kamuran Turksoy
(Illinois Institute of Technology)

Physical activity is one of the many factors that significantly affect blood glucose concentration (BGC) in patients with type 1 diabetes (T1D). The variations in BGC of a T1D depends on the intensity and duration of physical activity. The most common consequence is an increase in insulin sensitivity, which subsequently increases glucose uptake from the blood stream to tissue cells. When the exercise is prolonged or its intensity is increased, BGC can drop significantly, causing serious damages such as dizziness, unconsciousness, seizures, and if untreated, diabetic coma or death. Seeing this important and critical influence of physical exercise on BGC, a model that describes the relationship between glucose concentration and physical activity levels should be developed. Then, this model can be implemented into a closed-loop control system known as artificial pancreas that calculates optimum insulin amounts to keep BGC in target range ([1], [2]).

We use energy expenditure as an indicator of physical activity. To find the equation to predict the energy expenditure during exercise, a linear model for basal level of energy expenditure was developed based on subject's physical characteristics, such as weigh, height, gender and age. The basal or resting level of energy expenditure is the amount of energy per minute that the body needs to keep working, even though there is no physical exercise. Several exercise intensity intervals are defined and used as inputs of the model. The model predicts energy expenditure levels based on pre-defined intensity intervals.

There are many inputs that can be used to predict the energy expenditure during an exercise such as body acceleration, heart rate, oxygen consumption, and body temperature. However, only a few of them can be measured in real-time under daily living conditions and incorporated into an equation. The body acceleration is a good candidate and is being investigated to add as an input to the energy expenditure model to improve energy expenditure predictions.

[1] Turksoy, K., Bayrak, E. S., Quinn, L., Littlejohn, E., Cinar, A.. "Multivariable Adaptive Closed-Loop Control of an Artificial Pancreas Without Meal and Activity Announcement," *Diabetes technology & therapeutics*, 2013, 15(5), 386-400.

[2] Turksoy, K., Quinn, L., Littlejohn, E., Cinar, "A. Multivariable Adaptive Identification and Control for Artificial Pancreas Systems," *IEEE Transaction on Biomedical Engineering*, 2014. 61(3), 883-891.

3:00 PM (ThB3d) **MINEing Computationally Predicted Enzyme Promiscuity Products for Untargeted Metabolomics**

James Jeffryes (Northwestern University), *Ric Colasanti*
(Argonne National Lab), *Keith Tyo* (Northwestern University), *Christopher Henry* (Argonne National Lab)

In spite of its great promise, metabolomics has proven difficult to execute in an untargeted and generalizable manner. Liquid Chromatography-Mass Spectrometry has made it possible to gather data on thousands of intracellular chemicals. However, matching metabolites to their spectral features continues to be a bottleneck, meaning much of the collected information remains un-interpreted and that new metabolites are seldom discovered in untargeted studies. These challenges require new approaches that consider compounds beyond those available in curated biochemistry databases.

We present Metabolic In silico Network Expansions (MINEs), an expansion of known metabolite databases to include molecules that have not been observed, but are likely to occur, based on known metabolites and common biochemical reactions. We utilize an algorithm called the Biochemical Network Integrated Computational Explorer (BNICE) and expert-curated reaction rules based on the Enzyme Commission classification system to propose the novel chemical structures and reactions that comprise MINE databases. Starting from the Kyoto Encyclopedia of Genes and Genomes (KEGG) COMPOUND database, the MINE contains over 565,000 compounds of which 93.1% are not present in the PubChem database. However, these MINE compounds also have on average higher structural similarity to Natural Products (NP) than compounds from KEGG or PubChem. MINE databases were able to propose annotations for 98.6% of a set of 667 MassBank spectra, 14% more than KEGG alone.

MINE databases are freely accessible for non-commercial use via user-friendly web-tools and developer-friendly APIs. MINEs improve metabolomics peak identification as compared to general chemical databases whose results are diluted by synthetic compounds and complement previous in silico generated compound databases that focus on human metabolism.

3:15 PM (ThB3e) **Meal Detection Based on Qualitative Representation of Continuous Glucose Monitor Measurements**

Sediqeh Samadi, *Kamuran Turksoy*, *Ali Cinar* (Illinois Institute of Technology)

Type 1 diabetes (T1D) is a chronic metabolic disease in which patients suffer from hyperglycemia (high blood glucose concentration) because impaired insulin production prevents glucose transfer from the bloodstream to cells. Artificial pancreas (AP) control systems offer an important improvement in regulating blood glucose concentration of patients with T1D [1]. Accurate closed-loop control is essential for developing AP systems that adjust insulin infusion rates from insulin pumps [2]. For different AP control algorithms such as model-predictive control, adaptive control, and fuzzy logic control, meal information is a beneficial input to the controller. A controller including meal announcement has more reliable prediction of the actual change of blood glucose concentration. However, for a fully automated AP system, the meal information cannot be provided by users. Meal information must be derived from available process measurements such as continuous glucose measurement (CGM) signal and infused insulin values. The current work focuses on development of a meal detection algorithm that can be implemented into the AP control systems. Meals are detected based on qualitative representations of CGM and insulin infusion signals. In addition to qualitative representations, several heuristic rules are defined for prevention of wrong meal detections. The method is tested on different virtual patients data that are generated from the UVA/Padova metabolic simulator [3]. The preliminary results show that the proposed method eliminates the need of meal announcement and can provide a fully automated AP environment in terms of meal announcement.

[1] Turksoy K, Cinar A. Adaptive Control of Artificial Pancreas Systems - A review. *Journal of Healthcare Engineering* 2014, 5(1), 41–22.

[2] Turksoy K, Bayrak E.S, Quinn L, Littlejohn E, Cinar A. Multivariable Adaptive Closed-Loop Control of an Artificial Pancreas Without Meal and Activity Announcement. 2013, 15(5), 386-400.

[3] Kovatchev BP, Breton M, Dalla Man CD, Cobelli C. In silico preclinical trials: a proof of concept in closed-loop control of type 1 diabetes. *J Diabetes Sci Technol*. 2009;3(1):44-55.

3:30 PM (ThB3f) **Parameter Estimation in Cellular Systems Modeled as Stochastic Differential Equations**

Kirti M. Yenkie, Urmila Diwekar, Andreas Linninger (UIC)

The deductions of rate laws in cellular environments has always been a difficult task in the characterization of the systems behavior. The factors like low-dimensionality, high macromolecular content, spatial heterogeneity render the classical laws of mass action invalid. The reaction propensities vary at different times and their values are not easily determined using regular functions. Thus, the deterministic models cannot capture the true behavior and here the development and advancements in stochastic differential equation (SDE) modeling can play a major role.

Stochastic differential equations are widely used in disciplines like finance, engineering, environment, physics, population dynamics and medicine. The predictive power of SDEs lies in

the choice of the parameter values which can describe the real data effectively. Thus, the problem of finding an accurate and computationally feasible method for parameter estimation has been a key research area. Its importance has increased in recent years due to the application in wide range of fields like pharmaceutical problems, ecosystem models, medical data like EKG, blood pressure, sugar levels, wind and sound wave fluctuations, etc. The parameter estimation in SDEs is a well studied problem in literature, but most methods are time consuming, involve computational difficulties and at times result in objective functions which are non-differentiable. Our aim is to model cellular systems in the form of SDEs and use an appropriate Ito representation for their behavior. The SDE consist of two parts; the drift term or the deterministic part and the diffusion term or the stochastic component. We divide the parameter estimation problem in two levels; the inner level is the estimation of parameter (σ) due to randomness, usually addressed as the ‘standard deviation’ in the diffusion part and the outer level involves determination of parameters (θ) in the drift part.

In the suggested approach, σ is estimated by analyzing the available data and, thus, the parameter in the diffusion term is evaluated without any optimization or probabilistic methods. The parameters in the drift term (θ) are estimated by using kinetic inversion methods available for deterministic systems. However, instead of using the least square error minimization as the objective, the objective function is modified to include the parameter due to randomness. The results of the SDE are evaluated by using the estimated parameters in the model and solving the system for the expected value. The expected value is then compared with the actual data and the results from the deterministic model. The goal is to apply the proposed method to case studies like cellular pathways and metabolic models of different species and compare the SDE model projections and parameter estimates with deterministic models, stochastic simulation algorithms and conventional parameter estimation techniques to pave a new path in cellular systems modeling.

3:45 PM (ThB3g) **Parameter Estimation of Spatiotemporal Infectious Disease Models Using Nonlinear Dynamic Optimization**

Michael Bynum, Carl Laird (Purdue University)

In order for public health officials to make well-informed policies regarding infectious diseases, a solid understanding is required of not only the local spread of infection but also of transportation between cities. However, parameter estimation with infectious disease models considering transport between even a small number of cities can prove quite difficult. Many parameter estimation techniques, such as MCMC, become computationally prohibitive for these large, complex models. In this work, we show the effectiveness of nonlinear programming in the simultaneous estimation of both transmission parameters and transportation model parameters. A compartment model is used to represent the susceptible and infected classes. This model is comprised of differential

equations describing the birth, infection, and recovery processes. A gravity model is used to describe the transportation of infected individuals between cities. The resulting parameter estimation problem is a large-scale DAE constrained NLP.

The resulting NLP is modeled in Pyomo and solved with IPOPT, which uses an interior point algorithm designed for large-scale NLP's. The DAE is discretized using a three point Radau Collocation scheme. We show the effectiveness of the approach using data from stochastic simulations and real measles data from England.

4:00 PM (ThB3h) **A Hybrid Kinetic Model for Synthesis of Monoclonal Antibodies** by Hybridoma Cells *Denizhan Yilmaz, Satish J. Parulekar, Ali Cinar* (Illinois Institute of Technology)

Monoclonal antibodies (MABs) are important reagents used in biomedical research, in diagnosis and treatment of diseases. Monoclonal antibodies (MABs) derived from hybridoma cell cultures are used extensively in diagnostic assays and have found increasing use in therapeutic applications, affinity production systems, and in vivo imaging. The cell lines, hybridoma, are produced by fusing B cells (lymphocytes) from immunized animals with myeloma cells. The simplest approach for producing a MAB in vitro is to grow the hybridoma cells in batch and fed-batch cultures and recover and purify the MAB from the culture medium. The large scale production of MABs occurs via in vitro cultivation of hybridoma cell lines in bioreactors using techniques similar to those used for microbial cultivation. A cost-effective production of MABs requires an understanding of the effects of bioreactor process variables on the physiology of hybridoma cells. With this intention, a predictive kinetic model for hybridoma growth and Mab synthesis is developed in this work. The model is a hybrid of unstructured kinetics and structured kinetics. The unstructured component of the model describes utilization of glucose and glutamine for mammalian cell growth. Both of these nutrients promote cell growth. Mammalian cell growth is inhibited by lactate and ammonia, two products of cellular metabolism. The unstructured component of the kinetic model accounts for fates of glucose, glutamine, viable hybridoma cells, lactate and ammonia. The structured component of the hybrid kinetic model describes MAB synthesis by hybridoma cells. A reduced model for MAB production is obtained from the structured kinetics by invoking quasi-steady state assumption for all intermediates. Performance of batch, perturbed batch (intermittent addition of glucose and/or glutamine), and fed-batch cultures is simulated. The model predictions are in qualitative and quantitative agreement with experimental data reported in the literature for Immunoglobulin G (IgG) antibodies. These have been produced at a variety of scales, from small scale (2 L) to commercial production scale (15000 L) bioreactors. The effect of dilution due to cell growth in the structured kinetics component of the hybrid model is examined. Development of a simulator based on the hybrid

kinetic model as well as four other sets of kinetic expressions reported in the literature is also discussed.

Electrochemical Energy Conversion and Storage

Thursday, March 12, 2015 (Herman Lounge, ThB4)

Chair: *Nancy N. Kariuki* (Argonne National Lab)

2:15 PM (ThB4a) **The effects of Structure and Composition of Microporous Layer on Performance in Electrochemical Reduction of CO₂**

Byoungsu Kim, Febrian Hillman, Paul J.A Kenis (University of Illinois at Urbana-Champaign)

The increase of carbon dioxide (CO₂) in the atmosphere is known as one of the most significant contributors to global climate change. Electrochemical reduction of CO₂ into valuable chemicals using renewable energy is one approach to reduce CO₂ emissions and store otherwise wasted excess electrical energy generated from intermittent renewable sources. Gas diffusion electrodes (GDEs) have been applied to fuel cells as well as CO₂ reduction to enhance the rate of the electrochemical process. In this study, the effects of structure and composition of micro-porous layers (MPLs) within the GDE on performance in electrochemical reduction of CO₂ are investigated. MPLs were customized by the combination of carbon black with polytetrafluoroethylene (PTFE) or Nafion. Distinction between GDEs with and without MPLs was clearly shown, as MPLs act as a physical support for the catalyst layer. Moreover, the cathode performances with various MPLs reveal that the optimized amount of PTFE and carbon amount result in high levels of CO production while suppressing unwanted hydrogen evolution reaction. In the same way, optimizing the Nafion content in MPLs helps to promote CO production.

2:35 PM (ThB4b) **High-k Laminated Polymer Composites with Extremely Low Dielectric Loss for Embedded Capacitors**

Binghao Wang (Northwestern University), *Aijuan Gu* (Soochow University), *Tobin J. Marks, Antonio Facchetti* (Northwestern University)

High dielectric constant (high-k) materials are able to store plenty of Electric charges and balance the original electric field intensity, so they exhibit great potential in micro-electronic, electrical and bioengineering fields. Electric conductor/polymer composites exhibit a great potential because the low loading content ensures good processing characteristics and other merits of the polymers matrix. However, their high leakage currents and dielectric losses are the significant drawbacks that pose a serious challenge due to the huge energy consumption and high risk of service. Here, we designed and fabricated novel laminated polymer composites with unique macro- and micro-structure (asymmetric double-layer, gradient double-layer & multi-layer, and sandwich structure). They exhibit very high dielectric constant and extremely low dielectric loss. The outstanding dielectric behavior of the laminated composites is found to result from the reinforced space charge polarization and subdued leakage current.

2:55 PM (ThB4c) **Monolayer (Hydroxy)oxide-Metal
Bifunctional Electrocatalysts for Hydrogen Evolution
Reaction: A First-Principles Perspective**

Zhenhua Zeng, Joseph Kubal, Jeff Greeley (Purdue University)

In the present study, on the basis of detailed density functional theory (DFT) calculations, and using Ni hydroxy(oxide) films on Pt(111) and Au(111) electrodes as model systems, we describe a detailed structural and electrocatalytic analysis of hydrogen evolution (HER) at three-phase boundaries under alkaline electrochemical conditions. We demonstrate that the structure and oxidation state of the films can be systematically tuned by changing the applied electrode potential and/or the nature of substrates. Structural features determined from the theoretical calculations provide a wealth of information that is inaccessible by purely experimental means, and these structures, in turn, strongly suggest that a bifunctional reaction mechanism for alkaline HER will be operative at the interface between the films, the metal substrates, and the surrounding aqueous medium. This bifunctionality produces important changes in the calculated barriers of key elementary reaction steps, including water activation and dissociation, as compared to traditional monofunctional Pt surfaces.

The successful identification of the structures of thin metal films and three-phase boundary catalysts is not only an important step towards accurate identification and prediction of a variety of oxide/electrode interfacial structure-properties relationships, but also provides the foundation for rational design and control of 'targeted active phases' at catalytic interfaces. The successful design of bifunctional electrocatalysts that exploit these structures, in turn, could ultimately lead to advances in the development of alkaline fuel cells.

[1]. Surnev, S.; Fortunelli, A.; Netzer, F. P. *Chem Rev* 2012, 113, 4314.

[2]. Shaikhutdinov, S.; Freund, H.-J. *Annu. Rev. Phys. Chem.* 2012, 63, 619.

[3]. Subbaraman, R.; Stamenkovic, V.; Markovic, N. et al, *Science* 2011, 334, 1256.

[4]. Subbaraman, R.; Greeley, J.; Stamenkovic, V.; Markovic, N. et al, *Nat Mater* 2012, 11, 550.

[5]. Strmcnik, D; Stamenkovic, V. R.; Markovic, N. et al, *Nat Chem* 2013, 5, 300.

3:15 PM (ThB4d) **Probing the Synthesis and Structure of
Li₅FeO₄ (LFO) Cathodes in Li-ion Cells**

Chi-Kai Lin, Xiaoping Wang, Michael Krumpelt, Christopher Johnson (Argonne National Lab)

Introduction: The push for high capacity cathodes capable of Li storage greater than Li/TM (TM=transition metal) ratio of 1 in Li-ion batteries is extremely challenging. Considering Li₂MnO₃ (2Li per TM; 459 mAhg⁻¹ theoretical), we have shown [1], as well as others [2], that two lithiums per Mn can be extracted in an initial charge yielding practical capacities >320 mAhg⁻¹, but

this process occurs only above 4.5 V, and requires a material with high-surface area. Nevertheless structural changes occur in this cathode on the first charge, and the Li₂MnO₃ phase is lost due to lithium and oxygen removal, wherein the resulting material (i.e. 'MnO₂') does not possess good electrochemical reversibility.

Moving away from capacity limited layered Li(TM)O₂ requires exploring other crystalline structure types. The antiferroite family of Li₂O (Li₈O₄; enlarged unit cell) is an interesting option since transition metals can substitute for tetrahedral Li in the structure. Note that there are more available tetrahedral interstitials for close-packed oxygen atoms (total of two per O), than for octahedral sites (total of 1 per O) thereby providing a clue about which structure types to pursue. A representative example is Li₅FeO₄ (LFO) that features replacing a total of three lithium atoms in Li₈O₄ (enlarged unit cell) with one Fe atom (a trivalent charged cation; two vacancies are also created). This material, if electrochemically active could, in theory, provide 5 Li/Fe or ~ 867 mAhg⁻¹, if made reversible. Certainly redox on oxygen could be necessary in order to access all of this lithium and that remains a topic for exploration in hybrid Li-ion Li-oxygen cells [3].

In the earlier publication on LFO used as a lithium source for charged cathodes in Li-ion cells, we were able to demonstrate that a total of 4 lithiums can be extracted from the cathode material up to 4.4 V vs. Li metal. This provided a charge capacity of ~ 690 mAhg⁻¹ [4]. We revisit this material for Li-ion cells (sealed cells; no oxygen gaseous source) and are now focused on optimizing the synthesis process and to thoroughly characterize the electrochemical-chemical mechanism that occurs on the first charge in hopes of making the cathode reversible to supply 700 mAhg⁻¹ on discharge above 3 V which can lead to energy densities of ca. >2000 Whkg⁻¹.

Results: Through a number of experiments wherein the LFO synthesis was optimized for calcination temperature, lithium salt (and amount to account for Li evaporation), metal precursor, and atmosphere, we settled on a nano-Fe₂O₃ iron precursor, LiOH•H₂O as Li salt and argon atmosphere with programmed heating profile: 16 hours at 600°C and then 72 hours at 800°C. This led to a homogeneous pinkish gray powder that was phase pure by X-ray powder diffraction (JCPDS-75-1253). It was noted that the electrochemical activity is very susceptible to the presence of unreacted, or residual Li₂O (perhaps amorphous) on the surface of the LFO powder that creates a very strong base, which is very hygroscopic and difficult to handle in air. Incorporation of lithium is also hard to detect (by XRD methods) since Li-deficient phases Li_{1-x}FeO₄ also have an anti-flourite structure.

The electrochemical voltage profile of LFO is shown in Figure 1 for conventional (micron-sized Fe₂O₃ precursor) and a nano-Fe₂O₃ precursor. The over-potential is lower and the extractable capacity is higher for the latter (magenta line). The subsequent discharge to 1 V is also plotted. It is evident that the material is irreversibly converted over to another phase that only shows Fe(III/II) redox at lower voltages below 2.5 V.

Reversibility, however, is fairly good over subsequent cycles within a large voltage window between 4 and 1 V yielding ~230 mAhg⁻¹ (not shown).

A voltage window opening experiment was also conducted and better reversibility is seen up to 2 lithium cations suggesting that the following electrochemical reaction may take place:



In this reaction, strictly written formally with Fe(V) product likely does not exactly proceed, but is intended to be further explored both experimentally and theoretically validated [5]. Earlier XANES/EXAFS studies, do, however invokes the Fe(IV) redox state in the oxidation process [4]. Certainly oxygen redox (lattice peroxide formation) must also be ascertained in this electrochemical mechanism [6] and is the subject of our ongoing experimentation. These results, and are most recent findings to date will be presented in this talk.

Antifluorite Li₅FeO₄ presents an interesting material pathway and design model to high capacity and high energy battery systems and through careful scientific progress is expected to result in considerable advances in the knowledge of advanced Li-ion cathodes utilizing oxygen 2p orbital and metal d-states hybridization for charge storage.

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- [1]. C. S. Johnson et al. *Electrochem. Commun.*, 6, 1085 (2004)
- [2]. A. Robertson, P. Bruce, *Chem. Mater.*, 15, 1984 (2003)
- [3]. M. M. Thackeray et al., *J. Phys. Chem. Lett.*, 4, 3607 (2013)
- [4]. C. S. Johnson et al. *Chem. Mater.*, 22, 1263-1270 (2010)
- [5]. M. Chan et al., submitted (2014)
- [6]. S. Okuoka et al., *Scientific Reports*, 4, 5684 (2014)

3:35 PM (ThB4e) **GLAD-SAD Pt-Ni alloy/Ni Nanorod Electrocatalysts as Highly Active Oxygen Reduction Reaction**

Nancy N. Kariuki (Argonne National Lab), Mehmet F. Cansizoglu, Mahbuba Begum, Mesut Yurukcu, Fatma M. Yurtsever, Tansel Karabacak (University of Arkansas at Little Rock), Deborah J. Myers (Argonne National Lab)

Polymer electrolyte membrane fuel cells (PEMFCs) have drawn significant attention as alternatives to traditional power sources, especially in automotive applications, due to their high energy conversion efficiency, zero emissions, and system robustness [1]. However, the sluggish kinetics of oxygen reduction reaction (ORR) on the cathode demand a high loading of active platinum (Pt) or platinum-rich alloy catalysts [2], which increases the cost of PEMFC systems. Cost reductions can be achieved by increasing the ORR kinetics of platinum-based catalysts and by more efficient utilization of platinum component of the catalyst. In addition, the limited durability of standard and advanced ORR electrocatalysts, associated with corrosion of the catalyst particles and support

[3, 4], remains a major obstacle. The development of carbon-free catalysts could address degradation issues associated with the carbon support.

Relying on the high performance of thin film-based electrocatalysts [4], the design of thin continuous Pt or Pt-alloy layer on non-precious metal nanorod-patterned substrates as the catalyst support could result in catalysts with higher utilization, reduced Pt loading, and enhanced activity and stability. In this work, well-adherent and continuous Pt-Ni thin films, with several different molar ratios of Pt to Ni were deposited on Ni nanorods (NRs) by combining the glancing angle deposition (GLAD) technique [5] for the deposition of Ni-NRs and small angle deposition (SAD) technique [6] for the deposition of a thin conformal coating of Pt-Ni on the Ni-NRs (designated Pt-Ni@Ni-NRs). The Pt-Ni@Ni-NRs structures were supported on glassy carbon for evaluation of ORR activity using the rotating disk electrode technique and aqueous acidic electrolyte. These Pt-Ni@Ni-NRs catalysts showed superior specific- and mass-activities for ORR compared to PtNi nanorod catalysts [7] that were prepared using the GLAD technique.

- [1] B. Johnston, M. C. Mayo and A. Khare, *Technovation*, 25, 569 (2005).
- [2] H. A. Gasteiger, S. S. Kocha, B. Sompalli and F. T. Wagner, *Appl. Catal. B-Environ.*, 56, 9 (2005).
- [3] J. C. Meier, C. Galeano, I. Katsounaros, A. A. Topalov, A. Kostka, F. Schuth and K. J. J. Mayrhofer, *ACS Catal.*, 2, 832 (2012).
- [4] D. F. van der Vliet, C. Wang, D. Tripkovic, D. Strmcnik, X. F. Zhang, M. K. Debe, R. T. Atanasoski, N. M. Markovic and V. R. Stamenkovic, *Nat. Mater.*, 11, 1051 (2012).
- [5] T. Karabacak, G. C. Wang and T. M. Lu, *J. Vac. Sci. Technol. A*, 22, 1778 (2004).
- [6] T. Karabacak and T. M. Lu, *J. Appl. Phys.*, 97 (2005).
- [7] N. N. Kariuki, W. J. Khudhayer, T. Karabacak and D. J. Myers, *ACS. Catal.*, 3, 3123 (2013)

3:55 PM (ThB4f) **Non-Carbon Catalyst Supports for Polymer Electrolyte Fuel Cells**

Xiaoping Wang, Tammi Nowicki, Nancy Kariuki, Debbie Myers, Chi-Kai Lin, Yang Ren (Argonne National Lab)

The most commonly used electrocatalysts in polymer electrolyte fuel cells (PEFCs) are nanosized platinum or platinum alloy (Pt-M1M2) particles dispersed on high surface area, porous, conductive carbon black (e.g., Vulcan XC-72). Carbon has become the state-of-the-art support due to its good electrical conductivity (e.g., 2 S/cm for Vulcan XC-72) and chemical stability in the fuel cell environment. However, during extended PEFC operation, or load cycling, and start-up/shut-down, the carbon undergoes electrochemical oxidation to form surface oxides and CO₂, accompanied by catalyst (Pt or Pt-M) oxidation/dissolution[1-3]. The presence of Pt or Pt-M nanoparticles also accelerates the carbon corrosion[1]. As a result, Pt particles sinter into larger particles, accompanied by weakening of the interaction between Pt and the carbon support which results in the dislodging of Pt from the carbon

support[3-5]. These processes lead to the loss of electrochemically active surface area (ECSA) of the electrocatalysts, resulting in a decline in fuel cell performance. Carbon corrosion is especially problematic in the automotive application, where the frequent shutdowns result in localized potentials close to 1.0 V at the air/fuel boundary in the Pt/C anode of the PEFC and as high as ~1.5 V at the Pt/C cathode[6-7].

To improve the durability of electrocatalysts and PEFCs, more durable catalyst support materials than carbon black have been investigated or developed. They include more stable carbon forms such as graphitized carbon[8-9] and carbon nanotubes or nanofibers[10-11] and non-carbon supports such as conducting/semiconducting oxides[12-14], transition metal carbides[15], nitrides (mainly TiN)[16], and silicides (mainly TiSi₂)[17-19]. In this work, we report on our investigations of alternative transition metal silicides (TMSs) as PEFC cathode catalyst supports. The candidate support materials were identified by studying the chemical and electrochemical stability and oxygen reduction reaction (ORR) catalytic activity of seven TMSs. Various synthetic approaches including colloidal synthesis using different capping agents, strong electrostatic adsorption (SEA), and wet impregnation were explored to make the silicide-supported Pt catalysts (Pt/TMS) with the desired phase, composition, and microstructure. The effect of the support treatment was also studied. The properties of the prepared Pt/TMS catalysts were characterized using transmission electron microscopy (TEM), X-ray diffraction (XRD), temperature-programmed oxidation/temperature-programmed reduction (TPO/TPR), and rotating disk electrode techniques.

Select silicides showed the requisite electronic conductivity and promising stability against oxidative degradation. Further work is needed to improve the dispersion of Pt nanoparticles on the silicide supports to translate these materials into viable fuel cell catalysts.

- [1]. Z. Siroma, K. Ishii, K. Yasuda, Y. Miyazaki, M. Inaba, and A. Tasaka, *Electrochem. Comm.*, 7, 1153 (2005).
- [2]. L. Li and Y. C. Xing, *J. Electrochem. Soc.*, 153, A1823 (2006).
- [3]. Y. H. Liu, B. L. Yi, Z. G. Shao, D. M. Xing, and H. M. Zhang, *Electrochem. Solid State Lett.*, 9, A356 (2006).
- [4]. G. A. Gruver, R. F. Pascoe, and H. R. Kunz, *J. Electrochem. Soc.*, 127, 1219 (1980).
- [5]. Y. Y. Shao, G. P. Yin, Z. B. Wang, and Y. Z., Gao, *J. Power Sources*, 167, 235 (2007).
- [6]. C. A. Reiser, L. Bregoli, T. W. Patterson, et al., *Electrochem. Solid State Lett.*, 8, A273 (2005).
- [7]. Y. Ishigami, K. Takada, H. Yano, et al., *J. Power Sources*, 196, 3003 (2011).
- [8]. K. Miyazaki, H. Shirakata, T. Abe, et al., *Fuel Cells*, 10, 960 (2010).
- [9]. S. Zhang, Y. Y. Shao, X. H. Li, et al., *J. Power Sources*, 195, 457 (2009).
- [10]. J. B. Yang, G. Goenaga, A. Call, and D. J. Liu, *Electrochem. Solid State Lett.*, 13, B55 (2010).

- [11]. H. S. Oh, K. Kim, Y. J. Ko, and H. Kim, *Internat. J. Hydro. Energy*, 35, 701 (2009).
- [12]. H. Chhina, S. Campbell, and O. Kesler, *J. Electrochem. Soc.*, 154, B533 (2007).
- [13]. Y. Liu, A. Ishihara, S. Mitsushima, and K. Ota, *Electrochim. Acta*, 55, 1239 (2010).
- [14]. H. Chhina, D. Susac, S. Campbell, and O. Kesler, *Electrochem. Solid State Lett.*, 12, B97 (2009).
- [15]. M. Nie, P. K. Shen, M. Wu, Z. D. Wei, and H. Meng, *J. Power Sources*, 162, 173 (2006).
- [16]. I. C. Halalay, B. Merzougui, M. K. Carpenter, S. Swathirajan, G. C. Garabedian, A. M. Mance, and C. Mei, US Patent No. 7,622,216 (2009).
- [17]. B. Merzougui, I. C. Halalay, M. K. Carpenter, and S. Swathirajan, US Patent No. 7,767,330 (2010).
- [18]. B. Merzougui, I. C. Halalay, J. T. Johnson, G. C. Garabedian, M. P. Balogh, and S. Swathirajan, Pub. No. US/2008/0118818 A1 (2008).
- [19]. J. Wu, F. Xia, M. Pan, and X.-D. Zhou, *J. Electrochem. Soc.*, 159, B654 (2012).

Professional Development: Entrepreneurship Panel

Thursday, March 12, 2015 (Crown Room, ThB5)

Chair: *Nik Rokop* (Illinois Institute of Technology)

2:15 PM Panel on Entrepreneurship

Said Al-Hallaj (AllCell), *Bonnie Haferkamp* (Illinois Institute of Technology), *Raja Krishnan* (Technology Transfer Consultant), *Jason Zielke* (LocusView)

Said Al-Hallaj, PhD is the CEO and co-founder of All Cell Technologies LLC, and a Visiting Research Professor of Chemical Engineering at the University of Illinois at Chicago (UIC). Dr. Al-Hallaj earned his B.Sc and M.Sc in Chemical Engineering from Jordan University of Science and Technology (JUST) and a Ph.D in Chemical Engineering from the Illinois Institute of Technology (IIT). Said co-authored a book entitled "Hybrid Hydrogen Systems" and has published over forty peer reviewed journal papers. Said is the co-author of several issued patents and patent applications in the areas of renewable energy, energy storage and conversion and water desalination.

Raja Krishnan is a consultant to life science startup companies and to the IIT Technology Commercialization Office. He is also an adjunct faculty at IIT. Raja graduated from Steve Blank's Lean Launchpad Entrepreneurship Program for the Life Sciences at UCSF in December 2013. Raja also has 15+ years of experience in the pharmaceutical industry in various roles within formulation development, process development, scale-up and manufacturing. He has a strong understanding of the drug discovery and drug development process and also the regulatory perspective. He will also be participating in the new MATTER incubator as a mentor. Raja earned a B.S. in Chemical Engineering from Cornell University and an M.S. in Industrial Pharmacy/Pharmaceutics from Long Island University. He also gained a Regulatory and Quality Compliance Certification from Purdue University. He has authored several scientific poster

presentations at American Association of Pharmaceutical Scientists Annual Conferences.”

Jason Zielke is President/CEO and Co-Founder of LocusView. Jason is a proven technology and business executive who has played a significant role in the launch, development and success of several companies, including most recently as CEO and Co-Founder at LocusView. LocusView builds and integrates mobile applications for capturing field and infrastructure data from construction, inspection, surveying, maintenance and excavation crews in the utility and pipeline sectors. LocusView products are commercially available and have been deployed at utilities and municipalities tested and proven by several utilities and municipalities across the country, in nearly 10 states. Prior to joining Locus View Solutions, Jason was a co-founder, Senior Vice President and Chief Technology Officer of Clean Energy Trust, an organization that “launches, funds, and grows clean energy businesses”. At CET, he developed strategy, operations and personnel to grow the organization from a concept into an influential and well-funded company in 5 years. Prior to the Clean Energy Trust, Jason was a Venture Associate at Dillon Kane Group, a Chicago based private-equity and advisory firm, where he assisted with investment and acquisition transactions, and helped launch several new companies, including an aviation software company, an automated insurance underwriting platform, and a battery technology company that he co-founded, licensing technology from Argonne National Lab. During his tenure as Senior Architect at STA Group, Jason launched a new software platform and services using expert-based and big data approaches for the insurance industry. Previously he was a software developer in a number of industries including insurance, health care diagnostics, payment solutions, consumer technology, and consumer products. He began his career as a chemical engineer at UOP. He has a B.S in Chemistry from Southern Illinois University, an M.S. in Chemical Engineering from the University of Tennessee, where he was also research associate at Oak Ridge National Laboratory. He earned his MBA from The University of Chicago Booth School Of Business in Finance and Entrepreneurship.

Refining Strategies for Maintaining High Production

Friday, March 13, 2015 (Ballroom, **FrA1**)

Chair: *Martin Gonzalez* (BP)

9:30 AM (FrA1a) Relieving Unit Constraints with My First DMC Application

Carl Towner (BP)

Advanced control with DMC is an established technology and there are many experienced implementers around the world. With so many published success stories it is easy to forget that for every engineer using the technology there is always a first time. This is my story.

A distillate hydrotreater at the Whiting Refinery obtained additional processing capability as a result of a furnace pass balancing DMC. The DMC works to increase the output of the

individual pass control valves subject to constraints on more or less equal valve positions pass outlet temperatures and pass control valve differential pressures. DMC reduced the average pass outlet temperature differential from 25°F to 22°F and opened the furnace pass control valves from an average of 60% to 95%.

The controller is composed of 4 manipulated variables (MVs), the individual furnace pass inlet control valves. There are 18 controlled variables (CVs) which include the calculated difference between each of the control valve positions, pass outlet temperatures, and control valve differential pressures. A solid understanding of the process was required to identify economic drivers and work with operations to realize the benefits. Additionally the new advanced control engineer needs to have a basic understanding of the control system to navigate the system independently and build the appropriate interface points.

Physical investigation of the equipment controlled creates a better understanding of unmeasured disturbances that may severely impact the function of the advanced control scheme. For example, in this application one can't see how many burners are on and whether or not burners are plugged. This can have a big impact on how the CVs respond to the changes in MVs. Likewise the ambient temperature may play a role in whether or not instrumentation is likely to function – during commissioning one of the differential pressure transmitters on a pass froze up and gave a value of -0.2 psi. A field walk can help you to design the controller to deal with these problems rather than compound them.

Experienced APC help is a key requirement for implementing a new DMC application. There are so many steps and so many places to get hung up that a good idea can flounder and die without a knowledgeable guide to help you through the details of implementation. Even “simple” problems like the furnace pass balancing scheme give advantages to the refinery and good training to the new control engineer.

9:55 AM (FrA1b) Oxygen for Improved Refinery Utilization

David Lenhart (Praxair), *John Scalise* (Praxair)

Most refiners are familiar with the use of oxygen in the Fluid Catalytic Cracking Unit (FCCU) and Sulfur Recovery (SRU) plants. This presentation will discuss other uses of oxygen that can improve profitability of refineries and other chemical complexes. Specifically, how oxygen can be applied to improve the capacity of a fired heaters, including examples of operating heaters. Finally, a unique high temperature oxygen technology will be discussed. An application of this technology for the reduction of NOx and CO from process flue gases will be presented.

10:20 AM (FrA1c) Refinery Hydrogen Dynamics – Impact of Tight Oil and Shale Gas

Ken Chlapik (Johnson Matthey)

The presentation will address the issues facing Refinery Hydrogen plant operators as tight oil crudes and condensates

are becoming available to refiners. This needs to be balanced with shale gas availability providing low cost feed for refinery hydrogen plants to allow volume swell and enhanced H₂/bbl operation for some hydroprocessing units. In addition, I will address the dynamic of new hydrogen sources occurring in the US in response to shale gas availability and rapid petrochemical growth and how they can impact the future hydrogen availability in the US.

10:45 AM (FrA1d) **Safer and Smarter Catalyst Sulfiding**

Randy Alexander, Mike Robinson (Reactor Resources)

After a hydrotreater or hydrocracker catalyst change, the fresh oxydic catalyst must be activated by converting the metal oxides to sulfides. This process, often called "presulfiding", can be unpredictable and difficult to control due to the limited amount of data available to the engineer during the sulfiding step.

Reactor Resources has introduced a SmartSkid™ DMDS Injection System that addresses most of the deficiencies associated with catalyst sulfiding. The SmartSkid System is specifically designed to inject sulfiding chemicals into a hydrotreating unit as safely and accurately as possible. Each SmartSkid is also equipped with wireless telemetry, allowing customers to constantly monitor flow rate, total quantity injected, pressure, and temperature by accessing a secure web page

In addition, Reactor Resources has added an Online H₂S Analyzer System that continuously monitors the H₂S level of the reactor gas effluent. This data is also displayed with the pump telemetry and eliminates the hazardous ritual of operations personnel donning SCBA to pull draeger tubes.

Real time H₂S data is useful when controlling DMDS injection rates, minimizing the chance of over-injection that can lead to purging and excess sulfur emissions.

Advances in Catalysis

Friday, March 13, 2015 (Armour Dinning, FrA2)

Chair: *Christopher L. Marshall (Argonne National Lab)*

9:30 AM (FrA2a) **Fundamental Mechanistic Studies of Formic Acid Decomposition on Pd: Structure Sensitivity and Surface Coverage Effects**

Sha Li (University of Wisconsin Madison), Jessica Scaranto (SABIC), Srinivas Rangarajan and Manos Mavrikakis (University of Wisconsin Madison)

The catalytic decomposition of formic acid is of great importance not only because formic acid is a by-product derived with high concentrations in biomass reforming, but also because it can be used effectively as a fuel in fuel cells or as a hydrogen donor in catalytic transfer hydrogenation reactions. Pd represents one of the most active catalysts for formic acid decomposition and it is widely employed as anode in direct formic acid fuel cells. In this work, we studied the gas-phase decomposition of formic acid on Pd(111) and Pd(100) surfaces using first-principles density functional theory (DFT)

calculations. Minimum energy paths for HCOOH decomposition into CO₂ and H₂ (dehydrogenation products) or CO and H₂O (dehydration products) were analyzed and compared on the two Pd facets. It was found that CO₂ formation is more favorable than CO formation on clean Pd(111) surface while CO formation is more favorable on clean Pd(100) surface. On both facets, CO is produced mainly through the COOH intermediate instead of HCOO. We further studied this reaction on CO covered Pd(111) and Pd(100) surfaces as there is clear experimental evidence that CO is accumulated on Pd surfaces during the reaction. It turned out that the presence of CO not only changed the reaction energetics but also changed the minimum energy pathways for formic acid decomposition on both facets. Compared with clean surfaces, formic acid decomposition is more difficult in presence of CO on both facets. However, the effect of CO is more dramatic on (111) facet compared with (100) facet, which is more active than the (111) facet for formic acid decomposition when CO is present on the surface. This systematic mechanistic study of structure sensitivity and surface coverage effects of formic acid decomposition on Pd surfaces provides useful insights for vapor phase catalytic decomposition of formic acid, and should also be useful towards the understanding of electro-oxidation of formic acid on Pd by including the electrode potential and other important factors in assessing electro-catalytic decomposition of formic acid.

9:50 AM (FrA2b) **Synthesis and Evaluation of Highly Dispersed FeOx-CeO₂ Catalysts for NOx Reduction**

Justin Notestein, Dario Prieto-Centurion, and Louisa Savereide (Northwestern University), Charles Roberts and Paul Fanson (Toyota)

This talk will discuss the synthesis and evaluation of highly dispersed FeOx-CeO₂ catalysts for NOx reduction, as relevant to automotive emissions.

10:10 AM (FrA2c) **Systematic Study of Support Effects on Selective Hydrogenation of Acrolein**

Payoli Aich (UIC), Haojuan Wei (UIC), Christopher L. Marshall and Jeffrey T. Miller (Argonne National Lab), Randall J. Meyer (UIC)

A series of supported catalysts using three standard supports are prepared (SiO₂, Al₂O₃, and TiO₂) of different particle size to study the support effect on selectivity of acrolein hydrogenation towards allyl alcohol. We found with increase of basicity of a support the selectivity towards unsaturated alcohol increased. Also, on each support, a similar particle size effect on selectivity (bigger particle size, better selectivity) was observed. A detailed pathway analysis and kinetics study is currently underway on TiO₂ in an effort to understand the role of the support on catalyst performance. It is observed that the selectivity is as high as 88% at 1% conversion and then decreases to a stable 52% at 10% conversion. For both higher and lower conversions, the selectivity was better than our silver on silica catalyst of same size.

TiO₂ showed a prominent role in modifying the selectivity of the silver catalyst towards unsaturated alcohol. Formation of Ti³⁺ sites are believed to favor the adsorption of acrolein through carbonyl bond which is also confirmed by DFT calculations (Acrolein adsorbs more favorably (-0.99 eV) than olefinic bond (-0.45 eV)).

10:30 AM (FrA2d) **ALD Overcoating as a Means for Improving Catalyst Selectivity and Stability**

Christopher L. Marshall (Argonne National Lab), *Hongbo Zhang* (Argonne National Lab), *Peter C. Stair* (Northwestern University), *Jeffrey W. Elam* (Argonne National Lab), *Brandon O'Neill* (University of Wisconsin), *James A. Dumesic* (University of Wisconsin)

To provide more stable and active catalysts for processes such as biomass processing requires a method for controlling the synthesis of catalytic metals on the atomic scale. One such method, Atomic Layer Deposition (ALD), has been shown to be effective at controlling metal sites and improving catalytic activity, selectivity and longevity. ALD is a thin film deposition process which applies self-limiting or sequentially self-terminating films via chemical vapor deposition. ALD uses chemicals called precursors and alternating surface reactions to grow self-limiting layers of film. Some advantages of a self-limiting nature of ALD include uniform surfaces, high conformity to surface features, high control and accuracy of atomic level thickness, and high reproducibility. ALD provides a very controlled method in which atomically precise metal growth to a desired thickness is produced.

Recent work in our laboratories has found that overcoating active metals with materials such as Al₂O₃ or TiO₂ ALD can suppress the deactivation of a series of metals (Pt, Pd, Co, Cu) caused by sintering and leaching. In the current work, in situ and operando X-ray absorption methods were used to elucidate the mechanism of ALD overcoating of Cu nanoparticles and the effect of ALD overcoatings against vapor phase furfural reduction reactions over Cu-chromite. A factor analysis method was used to break down the XANES spectra into several components corresponding to different Cu states, and these were analyzed during the reductions. This presentation will provide insight into the reduction process of Cu-chromite before and after ALD treatment, and demonstrate that the ALD process can improve the stability of Cu-chromite catalysts in vapor phase furfural hydrogenation. Other examples of ALD overcoating will show that the material selectively preferentially binds to edge and corner sites which are non-selective leaving the selective planar sites available for catalysis.

10:50 AM (FrA2e) **Impact of Spatial Segregation in Catalytic Reactors – Two Identical Reactors with One-Way and Two-Way Interaction**

Satish J. Parulekar (Illinois Institute of Technology)

The effect of spatial segregation in catalytic reactors is mimicked by considering two well-mixed reactors with one-way

and two-way coupling. The reactors in the two-reactor system are identical only in terms of feed composition and reactor space time. The reactors need not have identical volumes and volumetric feed, effluent, and exchange rates. A comprehensive analysis of static and dynamic behavior of a catalytic reaction occurring in the two-reactor system is presented. The example considered pertains to a catalytic reaction exhibiting inhibition kinetics with respect to a reactant. Enzyme-catalyzed reactions subject to substrate inhibition belong to this class of reactions. A single well-mixed reactor may operate at up to three steady states. A two-reactor system may admit up to nine steady states at least at very low interaction rates. Three of these steady states, symmetric steady states, correspond to identical composition in the two reactors. The remaining steady states, the asymmetric steady states, correspond to different composition in the two reactors and are admissible over a range of interaction rates. Three different types of interaction are considered here: (1) equal interaction, (2) unequal interaction, and (3) one-way interaction (series reactors). The six asymmetric steady states exhibit four different pairing sets with two or more limit points. When the interaction rates are equal, the asymmetric steady states are comprised of sets of steady state counterparts, each set admissible over the same range of interaction rate. In terms of merges at limit points, the asymmetric steady states exhibit two pairing sets in the operating parameter space. A switching in steady state pairs is caused through emergence of four additional steady states, which are admissible over the same range of interaction rate. When the interaction rates are not equal, three pairs of asymmetric steady states are admissible over different ranges of interaction rates. In terms of merges at limit points, the asymmetric steady states exhibit three pairing sets in the operating parameter space, two inherited from the equal interaction rate case. The additional pairing set corresponds to the unique pairing set for one-way interaction between the two reactors. Two such pairing sets are possible depending on which of the two interaction rates is higher. The two switches in steady state pairs are caused through emergence of four additional steady states, which are admissible over two different ranges of interaction rates. The additional pairing set is admissible over a broader region of the operating parameter space as the inequity between the interaction rates is increased. The limiting case of this inequity corresponds to two reactors in series, where there is only pairing set of the asymmetric steady states and no additional steady states emerge. Numerical illustrations reveal the rich steady state structure of the reaction scheme in coupled reactors. The steady states are tracked systematically as the interaction rate is varied. The catalytic reaction exhibiting inhibition kinetics does not lead to periodic states in two-reactor systems. The two-reactor system is operationally more flexible and more robust vis-a-vis single reactor. Emergence of additional steady states at intermediate values of interaction rates reveals that the two-reactor system is an example of a complex system.

11:10 AM (FrA2f) **An Experimental and Theoretical Study of Glycerol Selective Oxidation to 1,3-Dihydroxyacetone via Bimetallic Platinum-Bismuth Catalysts**

Yang Xiao, Zhi-jian Zhao, Jeffrey Greeley, and Arvind Varma (Purdue University)

It is important to utilize glycerol, the main by-product of biodiesel production, to manufacture high value-added chemicals such as 1,3-dihydroxyacetone (DHA). In our prior work, a series of optimized Pt-Bi catalysts was prepared for selective oxidation of glycerol to DHA. The catalytic mechanism, however, remained unclear. In the present work, both experimental and theoretical approaches were used to reveal the DHA formation mechanism. Specifically, the performance of five different catalysts (Pt-Bi/AC, Pt-Bi/ZSM-5, Pt/MCM-41, Pt-Bi/MCM-41 and Pt/Bi-doped MCM-41) was investigated experimentally and Pt-Bi/MCM-41 exhibited the highest DHA yield. Using a periodic slab-model density functional theory (DFT), computations were made to obtain energy barriers of elementary steps, reaction pathways and Bi effect as an additive to Pt catalyst. Further, based on the DFT results, a micro-kinetic model was developed, which matched well with the experimental kinetic data, with no adjustable parameters. Both the experimental and calculated kinetics show that for high DHA selectivity, Bi should be placed on top of Pt, rather than inside or below Pt or in the support skeleton. The promoter effects of Bi, including electronic repulsion and steric hindrance, were identified for the DHA formation mechanism. The results demonstrate that the Bi species on the Pt surface is necessary and efficient to convert glycerol to DHA selectively.

Biomaterials

Friday, March 13, 2015 (Alumni Lounge, **FrA3**)

Chair: *Nancy W. Karuri* (Illinois Institute of Technology)

9:30 AM (FrA3a) **Agent-Based Modeling of Concurrent Biomaterial Scaffold Degradation and Vascularization**

Chenlin Lu (Illinois Institute of Technology), *Hamidreza Mehdizadeh* (Pfizer), *Elif Seyma Bayrak* (Amgen), *Sami Somo*, *Eric M. Brey*, *Ali Cinar* (Illinois Institute of Technology)

Biomaterial scaffolds are an important component in tissue engineering and regenerative medicine. They serve as a substrate for angiogenesis and tissue growth by providing mechanical and structural support required for appropriate cell function and morphogenesis. The degradation behavior of scaffolds affects angiogenesis significantly since it changes the porous structure and mechanical properties of the scaffold dynamically over time. It is important for the scaffold to degrade at a balanced rate and maintain the scaffold integrity during the tissue formation. One problem that may arise during the biological process is the mechanical failure of the tissue

engineering construct as a result of fast scaffold degradation before production of new tissue.

An agent-based model (ABM) of biomaterial scaffold vascularization is extended to consider the effects of scaffold degradation on the dynamics of angiogenesis [1]. The research is focused on the investigation of the combined effects of scaffold porous architecture and degradation on vascularization process. A statistical model developed by Metters et al. to describe the bulk degradation of PLA-b-PEG-b-PLA hydrogel is used to incorporate scaffold degradation into the ABM [2]. The degradation rate of scaffolds can be manipulated and altered based on the degree of crosslinking, polymer composition, and/or polymer concentration. A multi-layer scaffold model having regions with different degradation rates within the scaffold structure was designed. Simulation with multi-layer scaffolds show that vascularization was successfully continued after the previous layer was fully disintegrated because a considerable portion of the present layer was still remaining and providing sufficient mechanical strength and cell-attachment sites for angiogenesis. Simulation results indicated that the multi-layer scaffold model can optimize the vascularization without losing mechanical support of the biomaterial scaffolds.

The simulation results indicate that scaffold degradation plays an important role in angiogenesis, especially, when the initial overall porosity of the scaffold is low. Also, degradation is more effective and improves vascularization more in scaffolds with smaller pore sizes compared to those having larger pore sizes. In general, it is observed that degradation can be utilized as a means of enhancing vascularization in scaffolds in which angiogenesis happens slowly and is limited to insufficient depths. These results can be used in combination with experimental research to design optimal scaffold structures. [1]. H. Mehdizadeh, S. Sumo, E.S. Bayrak, E.M. Brey, A. Cinar, "Three-dimensional modeling of angiogenesis in porous biomaterial." *Biomaterials*, 34(12), pp.2875-2887, January 2013.

[2]. A.T. Metters, C.N. Bowman, K.S. Anseth, "A Statistical Kinetic Model for the Bulk Degradation of PLA-b-PEG-b-PLA Hydrogel Networks." *J. Phys. Chem. B*, 104(30), pp.7043-7049, July 2000.

9:45 AM (FrA3b) **Proteolysis of Decellularized Extracellular Matrices Generates a Significant Amount of Fibronectin Fragments**

Anand Ramanathan, Nancy W. Karuri (Illinois Institute of Technology)

Fibronectin degradation has been closely associated with a number of pathologies ranging from periodontal disease to wound repair and cancer. Excessive inflammation in the wound is believed to result in increased fibronectin proteolysis and impaired wound healing. We studied the impact of fibronectin degradation on decellularized extracellular matrices. These were treated with alpha chymotrypsin and proteolysis stopped at different time points. The content of the protease solution

as well as that of the immobilized matrices was examined by immunoblotting and Bicinchoninic Acid assays. Fibronectin was 5.0% of the total decellularized matrix but was extremely susceptible to proteolysis; after 15 minutes of protease treatment 62 % of the fibronectin in the decellularized extracellular matrix was fragmented while there was an 11.1% decrease in the total protein in the extracellular matrix. A cell adhesion assay was used to quantify NIH 3T3 mouse fibroblast adhesion, spreading and actin extensions when seeded on the decellularized extracellular matrices at the different time points of proteolysis. Cell number, cell area and actin extensions within the extracellular matrix decreased with increased proteolysis time. The protease solutions containing fibronectin fragments were coated on glass cover slips and cell adhesion and spreading were monitored. Cell adhesion and spreading increased with the concentration of fragments in the protease solution. This study demonstrates that in a high protease environment, fibronectin in the extracellular matrix is more susceptible to fragmentation than the total extracellular matrix protein content and places weight on bioengineering strategies to stabilize fibronectin against proteolytic fragmentation as a therapeutic strategy.

10:00 AM (FrA3c) **Substrate Stiffness Influence on Adipose Tissue Expansion and Function**

Marcella Vaicik (Illinois Institute of Technology), *Ronald Cohen* (University of Chicago), *Jose Rios*, *Georgia Papavasiliou*, and *Eric M. Brey* (Illinois Institute of Technology)

Obesity results in a greater than \$190 billion annual burden on US healthcare. The negative effects of obesity may outweigh the positive effects of smoking cessation on the overall health of the population. A number of soluble hormones and growth factors have been shown to have an influence on adipose tissue insulin sensitivity and expansion. However, little attention has been paid to the contribution of cell interactions with the extracellular matrix (ECM). The goal of this research was to develop a 3D culture model for the study of adipose-ECM interactions. We used poly(ethylene glycol) (PEG) hydrogels to study adipose expansion in 3D culture. PEG hydrogels offer a controlled environment for the study of substrate mechanical, physical and chemical properties. Hydrogels were prepared with various mechanical and chemical features and used for preadipocyte culture and differentiation. Using uniaxial compression testing we found that we could generate hydrogels with mechanical properties consistent with normal adipose tissue (2-32 kPa). The cells were able to differentiate and lipid load, independent of scaffold properties. In the absence of scaffold degradation, the rate of cell expansion varied with mechanical stiffness but not presence of cell binding sequences. Cells were maintained as a stable, viable and functioning adipose tissue mass for more than 20 days of culture in the non-degradable hydrogels even in the absence of cell adhesion sites. Current work is focusing on characterizing the metabolic function of these model

adipose tissue microcultures based on varying substrate properties. We have developed a method for long-term 3D culture of adipose tissue for the study of tissue function and screening of therapeutic interventions.

10:15 AM (FrA3d) **Agent-Based Simulation of Growth Factor Releasing Biomaterials**

Nan Xiao, *Elif S. Bayrak*, *Banu Akar*, *Hamidreza Mehdizadeh*, *Sami Somo*, *Eric M. Brey*, *Ali Cinar* (Illinois Institute of Technology)

Angiogenesis is an essential physiological process in tissue engineering where new blood vessels are formed from pre-existing vessels. Angiogenesis is influenced by the transport of various chemoattractants such as vascular endothelial growth factor (VEGF). VEGF is essential for migration, proliferation and survival, of endothelial cells. However, VEGF has a relatively short biological half-life, and overdoses can cause harmful side effects. Porous biodegradable polymers preloaded with growth factors are widely used in tissue engineering applications to provide both mechanical support and sustained localized growth factor delivery. However, there are still many technical challenges in obtaining satisfied controlled delivery in scaffolds in in vitro/vivo experiments. Agent-based modeling (ABMs) provides an economical and efficient option for simulating angiogenesis to understand and optimize this complex biological system. We have previously developed an ABM to simulate angiogenesis in 3D scaffolds with well-defined pore architectures (Mehdizadeh, Sumo et al. 2013). In this study, this ABM was extended to test the effects of different growth factor gradients by adjusting VEGF release rate. Important evaluation criteria for vascularization of scaffolds such as anastomosed depth, vessel invasion depth, total blood vessel length and density were reported. The results showed that sustained delivery of VEGF can support endothelial cell survival and enhance angiogenesis. This study also illustrated that ABMs can help in vitro/in vivo experimental research in the design of biomaterials with optimal structure and chemical properties to increase angiogenesis.

10:30 PM (FrA3e) **Ceramic-Hydrogel Composites Augment Bone Regeneration in a Rodent Critical Size Defect Model**

Banu Akar (Illinois Institute of Technology), *Shu-Wei Kao* (Chang Gung Memorial Hospital), *Katerina Stojkova* (Illinois Institute of Technology), *Ming-Huei Cheng* (Chang Gung Memorial Hospital), *Eric M. Brey* (Illinois Institute of Technology)

Bone defects arising from trauma, congenital abnormalities and tumor removal present major challenges to reconstructive surgeons. Current clinical methods are often insufficient for reconstruction of large defects. Tissue engineering has shown promise for regeneration of bone defects. Previous studies have suggested that the incorporation of ceramics like hydroxyapatite (HA) and tri-calcium phosphate (TCP) into hydrogel systems promotes bone mineralization. Recently, we have developed a method to generate composite porous

hydrogels with ceramics, which promotes bone tissue formation in vivo.

Degradable porous hydrogels with fibrin were produced using a particulate leaching method [1]. Hydrogel structure was composed of polyethylene glycol-diacrylate (PEG-DA) and PEG poly (L-lactic acid)-DA (PEG-PLLA-DA). Varying ratios of HA: TCP (0:0, 70:30, 50:50, 30:70 %) was incorporated into hydrogel structure to evaluate the optimum ratio of these ceramics for bone regeneration.

In this study, in vitro and in vivo degradation characteristics and mechanical properties of the system were investigated. The addition of ceramics in hydrogels can serve as the neutralizing agents on the acidic pH caused by the degradation by-products of the polymers. Therefore, HA and TCP included hydrogels exhibited relatively longer degradation times than controls (greater than 8 weeks).

A rodent cranial defect (critical size) model was used to examine the effect of HA and TCP on bone tissue regeneration. Animals were sacrificed at 4 weeks and 8 weeks. Micro-CT (Computed Tomography) was performed to image harvested samples and regenerated bone volume was quantified based on micro-CT images. Tissue structure was evaluated with histological stains. HA and TCP combined groups showed significantly higher bone regeneration than the control group. The highest bone replacement was found in the composite hydrogel (50:50, HA: TCP) at 8 weeks, which was around 75% of the total defect volume. Our results indicate that supplementing hydrogels with HA and TCP enhanced bone regeneration. We are currently examining the histological results.

[1]. Jiang, B., Akar, B., Waller, T. M., Larson, J. C., Appel, a a, & Brey, E. M. (2014). Design of a composite biomaterial system for tissue engineering applications. *Acta Biomaterialia*, 10(3), 1177–86. doi:10.1016/j.actbio.2013.11.029

10:45 AM (FrA3f) **Gradient Scaffolds for Vascularized Tissue Formation**

Yusheng He, Georgia Papavasiliou (Illinois Institute of Technology)

A critical criterion for the success of tissue engineered constructs is the ability to stimulate neovascularization (new blood vessel formation) upon implantation in order to mediate transport of oxygen and nutrients and removal of waste products. The process of neovascularization is highly dependent on gradients of soluble (chemotactic) and immobilized (haptotactic) extracellular matrix signals as well as gradients of matrix physical structure and mechanical properties (durotactic cues). While various engineering approaches have been exploited for the creation of gradients within 3D scaffolds, cell responses have been limited to 2D surfaces or to 3D invasion in response to gradients of a single factor. The creation of scaffolds with tunable simultaneous gradients of physiologically relevant chemotactic, haptotactic and durotactic cues on 3D vessel assembly has yet to be explored. We have previously developed a

photopolymerization technique (perfusion-based frontal photopolymerization (PBFP)) that allows for the creation of simultaneous gradients of haptotactic (cell adhesion ligand concentration and protease-sensitive peptide domains) and durotactic (elastic modulus and swelling ratio) in poly (ethylene glycol) (PEG) hydrogel scaffolds. The goal of the present study is to decouple chemotactic, haptotactic and durotactic gradients in hydrogel scaffolds in order to systematically determine the role of each of these gradients in vessel assembly. Manipulation of the composition as well as the flow rate and duration of specific prepolymer components during PBFP, allows for the creation of hydrogel scaffolds with decoupled gradients. Using this approach, scaffolds with immobilized gradients in the YRGDS cell adhesion peptide ranging 30-120 μM over a length of 1 cm, were created while maintaining a uniform elastic modulus and swelling ratio. Current studies are aimed at using this approach to create scaffolds with independent and combined gradients of chemotactic, haptotactic and durotactic cues in order to explore their role on 3D in vitro vascular sprout invasion.

11:00 AM (FrA3g) **Fibronectin Matrix Degradation by α -Chymotrypsin**

Xue Geng, Yaozhu Leng (Illinois Institute of Technology)

Our project is focus on the protease (α -chymotrypsin)'s influence on fibronectin (FN) matrix with different time and concentrations. For this purpose, we first got cell free matrix and using Florescence Microscope proved the intact of FN matrix. Then FN were deal with α -chymotrypsin with different designed time to monitor the proteolysis of matrix FN. The time period was from 0 to 30 at 5 minutes interval. We also repeated different time proteolysis by using two concentrations of α -chymotrypsin, which were 1 $\mu\text{g}/\text{ml}$ and 5 $\mu\text{g}/\text{ml}$. By using immunofluorescence before 0 minute and after 30 minutes of proteolysis show that FN' structure has been affected by α -chymotrypsin. After the degradation the fibronectin by protease in different time, we load the samples into SDS-PAGE, and then doing silver stain and western blot, in order to figure out what size and volume will be the α -chymotrypsin work on the FN. Therefore, two main results will be showed: one is the comparison of low and high concentration of protease. Another one is the influence of time under the same concentration of protease. The actual data showed as the time increase, fibronectin was degraded more completed. And compare with the lower group, higher concentration group showing a positive increase of degradation.

11:15 AM (FrA3h) **Cell Deprivation: Nutrient Limitation and Gene Knockouts of Escherichia Coli towards Enhancing Non-Growth Metabolism for Metabolic Engineering Purposes**

Will Bothfeld, Jennifer Greene, Divya Tikkavarapu, Grace Kapov, Keith Tyo (Northwestern University)

Gene overexpression or knockdown and heterologous pathway construction are the tools Metabolic Engineers first turn to when creating platforms for the production of chemicals and medicines. These strategies burden cells and can lead to diminishing productivities. Carbon and energy are wasted on unnecessary biomass during the chemical production phase and genetic deletions are limited to non-essential enzymes. Decoupling cell growth from product formation is one work around. However, stationary cells have drastically reduced metabolism. Increasing metabolism is one attractive platform for future metabolic engineering. We use a combination of nutrient limitation and auxotrophic gene deletions to characterize glucose flux and product secretion in *E. coli*; towards developing a catalytically active, non-growing cell. To modulate growth and production phases, native nutrient sensing is integrated into the classic genetic toggle switch circuit, to dynamically control the expression of pathway enzymes to produce polyhydroxyalkanoates.

Process Safety and Occupational Health

Friday, March 13, 2015 (Herman Lounge, **FrA4**)

Chair: *Brenton L. Cox* (Exponent)

Co-Chair: *Janet A. Grezlik* (PSRG Inc.)

9:30 AM (FrA4a) Lessons Learned from PSM Auditing and OSHA's Plans for Change

Bob Weber (PSRG Inc)

Auditing is one of the 14 elements under the Process Safety Management Standard (PSM). It is a critical element that assesses the effectiveness of an organization's PSM program and analyzes compliance with the PSM standard. Organizations can improve process safety management programs by an effective auditing program and from lessons learned. This presentation describes findings statistics and provides a guide to assessing an organization's PSM effectiveness and the changes OSHA plans to make in the future of auditing.

9:50 AM (FrA4b) Hazards Inherent to Batch Processing: Lessons Learned from Case Studies

Brenton L. Cox, Sean J. Dee, Andrew R. Carpenter, Russell A. Ogle (Exponent)

When considering whether to operate a process in batches or continuously, many considerations may inform the decision, such as technological capability, product yield and purity, and capital costs. Additionally, process technologies are often initially designed in batch mode at the laboratory scale. Intermittent product demand or feedstock availability can also be a strong driver toward batch manufacturing. However, when deciding between batch and continuous processing, the stakeholders must also consider hazards in batch processing that do not exist or are more easily limited in a continuous process.

For example, batch processes may require large inventories of hazardous feedstock or intermediates, whereas continuous processes may allow for "just-in-time" production. Chemical

reactivity may also vary widely at different stages of the batch. Material integrity may be tested as equipment can experience a wide range of operating conditions throughout a batch. Process control and safety systems may also present unique challenges in batch processes, e.g., a heat exchanger may serve to both heat and cool the same medium at different stages, while also being the first line of defense to quench a runaway reaction. Finally, batch processes often require a far greater degree of discrete process control logic (e.g., opening and closing valves, turning electric motors on and off, or starting or stopping material flows into a vessel) implemented either manually by operators or automatically using programmable logic controllers (PLCs). Thus, batch processes offer many more opportunities for human error.

To highlight these hazards, we examine case studies where circumstances unique to batch processing led to process upsets.

10:10 AM (FrA4c) Ignition of Flammable Vapors in Partially Filled Containers

Sean J. Dee, Brenton L. Cox, Russell A. Ogle (Exponent)

Containers partially filled with flammable liquids create a unique safety hazard during transfer, storage, and usage. In addition to the concerns regarding the safe handling of the liquid phase, the vapor headspace above the liquid also presents a potential flammability hazard. Depending on the physical properties of the flammable liquid, the fuel vapor concentration can fall within the range of flammability. For example, this hazard occurs with alcohols such as methanol, ethanol, and propanol.

If exposed to an ignition source, flammable vapor ignition can propagate back to the container and cause the expulsion of ignited flammable liquid from the container. In this work, several case studies will be presented that demonstrate this potential hazard. Then, calculations examining the impact of vapor pressure, flammability limit, and container fill volume for a variety of liquids will be presented as a method for evaluating the potential hazard. Finally, recommendations based on review of relevant standards and industry guidelines will be presented for safe handling and use of flammable liquids and vapors.

10:30 AM (FrA4d) Discrepancies in Methods for the Predicting the Explosion Energy of BLEVEs

Ronald Pape, Amy Richards, Michael Hanks (Engineering Systems Inc.)

BLEVE stands for Boiling Liquid Expanding Vapor Explosion. Birk (1) defines BLEVE as "the explosive release of expanding vapor and boiling liquid when a container holding a PLG fails catastrophically." A broader definition includes the catastrophic release of any liquid that is stored under pressure at a temperature that is substantially above its boiling point at atmospheric pressure. The liquid doesn't have to be a PLG. BLEVE can occur any time a liquid substantially above its boiling point at atmospheric pressure is catastrophically released as

the result of total loss of containment. No combustion has to be involved in the BLEVE process. However, many times BLEVEs are the result of a flammable liquid with the container "cooked" in a fire, heating the contents and weakening the container to the point of failure, resulting in the catastrophic release of the liquid, with the subsequent ignition of the dispersed flashing flammable liquid and vapor producing a fireball. Although in these cases a flash fire and fire ball results, the ignition and fireball are not per se part of the BLEVE. There is not universal agreement as to the mechanisms involved in a BLEVE, particularly concerning what drives the air blast pressure wave. There are also major differences in the models used to predict the explosion energy driving the blast wave. The authors have used calculation methods described in the CCPS book Guidelines for Vapor Cloud Explosion, Pressure Vessel Burst, BLEVE and Flash Fire Hazards, August 2010 and most recently similar methods in the PHAST process industry hazard analysis/consequence analysis software tool, developed by DNV GL. These models consider the explosion energy to be the energy difference between the thermodynamic state of the liquid at the time of loss of containment and the final state of that material when it expands to atmospheric pressure. The CCPS method includes a separate parallel calculation for the material initially in the vapor state in the container before loss of containment. Recently, Birk has compared various prediction methods to experimental data for propane BLEVEs and concluded that the flash vaporization of the liquid may be too slow to contribute significantly to the blast, and the blast energy is primarily from the vapor expansion. Ogle and coworkers have discussed the available energy using Exergy and compared this to the prediction methods of Prugh, CCPS and Planas. These various approaches can lead to drastically different predictions of explosion energy. The different BLEVE theories and models will be discussed and compared to existing experimental data using propane as the primary example.

10:50 AM (FrA4e) **Scaling Analysis for Confined Dust Flame Propagation**

Russell A. Ogle, Brenton L. Cox, Sean J. Dee (Exponent)

Dust explosions pose a threat to both people and property in any industry where combustible dusts are handled. A dust explosion is a multiphase reactive flow, specifically, a flame that propagates through a dust cloud. Spherical test vessels like the 20L and cubic meter sphere vessels have become the standard means for evaluating combustible dust hazards and for extracting data for the design of explosion protection systems. The fundamental assumption underlying the analysis of dust explosibility data is the thin flame approximation, i.e., the assumption that the dust flame thickness is much less than the characteristic dimension of the test vessel. The thickness of a dust flame is determined by the interplay between chemical kinetics and transport phenomena. Unlike premixed gas flames, thermal radiation can play a dominant role in dust flame propagation depending on the optical thickness of the dust cloud. This investigation uses scaling analysis to examine the

limits of the thin and thick flame approximations for laminar dust flame propagation in closed vessels.

11:10 AM (FrA4f) **Managing Change – Hurdles of the Past and Innovation for the Future**

Oleg Yazvin and Eric Allen (Environmental Intellect)

Management of Change (MOC) is a requirement mandated under OSHA's process safety management (PSM) regulation. Thousands of US operating facilities, spanning from refineries to food manufacturing industries are impacted by this requirement. It is generally a challenge to manage frequent and ongoing operational challenges at these types of facilities, especially given industry standard software and data systems that are employed. Though the advent electronic MOC programs like E-MOC and KMS have streamlined the process of managing approvals and archiving required checks, neither of these systems is capable of automating management system updates impacted by MOC. For example, a MOC at a petroleum refinery may result in the addition of a new flow transmitter for a flare gas line. This singular change impacts multiple management systems, including data historians, which will manage the data generated by a PI tag associated with that flow transmitter. Additionally, this change will impact the I&E equipment database, as well as environmental compliance systems. Ei has developed a fully electronic system that is capable of auto-updating each of these systems through database integration.

The authors will present common industry challenges with MOC as well as how Ei's technology is being implemented to improve efficiency and compliance workflow associated with MOC to meet the needs of the modern-day facility.

Advances in Optimization I

Friday, March 13, 2015 (Crown Room, FrA5)

Chair: *Carl Laird* (Purdue University)

9:30 AM (FrA5a) **Large-Scale Multi-Objective Multi-Stackholder Optimization**

Victor Zavala (Argonne National Lab)

We present a framework to solve multi-objective optimization problems in which the the opinions on priorities on objectives and constraints of multiple stakeholders are factored in the decision. We discuss applications in sustainable operations and model predictive control.

9:50 AM (FrA5b) **Efficient Ant Colony Optimization (EACO) Algorithm for Large Scale Optimization Problems**

Berhane H. Gebreslassie and Urmila M. Diwekar
(Vishwamitra Research Institute)

An efficient ant colony optimization (EACO) is a new metaheuristic optimization algorithm for tackling linear, nonlinear and mixed integer nonlinear programming problems. Initially, ACO has been practiced with great success for combinatorial optimization problems. In recent years, the research focus has extended from the combinatorial ACO

algorithm to continuous and mixed variable nonlinear programming problems. In this work, a new variant of ACO algorithm for deterministic optimization problems is proposed. In the proposed algorithm, an efficient sampling technique, Hammersley sequence sampling (HSS), is implemented to initialize the solution archive and to generate multidimensional random number for the transition probability test. Nine benchmark problems with 10 experiments for each benchmark in total 90 experiments are tested. In more than 99% of the total experiments, the results show computational efficiency improvement that range from 3% to 71%. Thus, this new method variant of ACO algorithm can be a useful tool to solve large-scale optimization problems. Finally, we investigate how the EACO algorithm performs on a real-world case study of solvent selection optimization problem.

Solvent selection is an important step in process synthesis, design, or process modification. The computer-aided molecular design (CAMD) approach, which is based on the reverse use of group contribution method, provides a promising tool for solvent selection. The existence of a combinatorial search space in molecular design poses a challenge for traditional deterministic optimization methods. In this work, we present a new approach to solvent selection using the EACO algorithm. An acetic acid extraction from waste stream of water based on the infinite dilution activity coefficient model is optimized. The UNIFAC model is used to estimate the mixture properties. As deterministic optimization technique, the EACO algorithm outperforms the conventional ACO, simulated annealing and genetic algorithm optimization techniques. New solvents with better targeted properties are proposed.

10:10 AM (FrA5c) **Multi-agent Optimization Framework to Solve Large Scale Process System Engineering Problems**

Berhane H. Gebreslassie and Urmila M. Diwekar
(Vishwamitra Research Institute)

The multi-agent optimization framework provides a way of combining various algorithms in one platform and exploits strength of each algorithm possesses. Large scale process system engineering problems are non-convex problems and such an approach avoids the problem of getting stuck in local optima as well as reduces the computational burden. In this work, we propose a multi-agent optimization framework for solving complex large scale process system engineering problems. The framework uses a variety of different algorithmic agents which include the gradient based local optimizers and heuristic algorithms; We investigates the effect of cooperation among agents of the agent-system working in parallel and combined into a framework designed to solve large scale combinatorial optimization problems. Computational experiments are carried out using benchmark problems and real world case study. The proposed methodology enables to improve the quality of solutions and the computational efficiency in comparison with non-cooperative and standalone agents. We have also examined solving the optimization problems with cooperative homogenous and heterogeneous

agent systems and the results indicate that the computational efficiencies are improved when the agents are heterogeneous. Moreover, the analysis of the intra- and inter agent cooperation show that depending the complexity of the problem the inter- and intra-agent collaboration has a significant impact on system performance.

10:30 AM (FrA5d) **Clustering-Based Preconditioning for Stochastic Programs**

Yankai Cao and Carl Laird (Purdue University), *Victor Zavala* (Argonne National Lab)

We present a clustering-based preconditioning strategy for KKT system arising in two-stage stochastic programming within an interior-point framework. This problem class arises in stochastic optimal control, robust design, and parameter estimation and has the property that an arrowhead block representation of the KKT system can be obtained. Each block corresponds to a scenario, which is typically obtained by sampling a probability distribution. The key idea is to perform adaptive clustering of scenarios inside the solver based on their influence on the problem. This results in a much smaller compressed KKT system and the compressed KKT system is used as a pre-conditioner for the full space KKT system. We derive spectral and error properties for the preconditioner. We also describe the features of our implementation in C++, demonstrate that scenario compression rates of up to 87% are possible, and that speedups of an order of magnitude are achievable. Finally, we demonstrate that the parallelization can push the performance further.

10:50 AM (FrA5e) **Globally Optimal Sensor Network Design Revisited: Application of the Generalized Bender Decomposition**

Jin Zhang, Donald J. Chmielewski (Illinois Institute of Technology)

In a series of papers [1, 2, 3] the problem of optimal sensor selection for linear systems has been shown to be of the Mixed Integer Convex Programming (MICP) class. While the use of such formulations has opened the door to a guarantee of global optimality, the use of a branch and bound search procedure has limited application of this approach to fairly small systems. The particular bottleneck can be attributed to the fact that during each iteration of the branch and bound search a fairly slow Semi-Definite Programming (SDP) problem needed to be solved to it global optimum.

In this work, we illustrate that a simple reformulation of the MICP and subsequent application the Generalized Benders Decomposition (GBD) will result in massive reductions in computational effort. While the resulting algorithm must solve multiple Mixed Integer Linear Programs (MILPs), this increase in computational effort is significantly outweighed by the reduction in the number of SDP problems one must solve. The approach will be illustrated using steady-state type processes (that use data reconciliation based estimation) as well as closed-loop dynamic process (that Kalman filtering based

estimation).

[1]. Chmielewski D. J., T. Palmer and V. Manousiouthakis, "On the Theory of Optimal Sensor Placement," *AIChE J.*, 48(5), pp 1001-1012, (2002).

[2]. Peng, J.K., and D.J. Chmielewski, "Covariance Based Hardware Selection-Part II: Equivalence Results for the Sensor, Actuator and Simultaneous Selection Problems," *IEEE Trans. Cont. Sys. Tech.*, 14(2), pp 362-368, (2006).

[3]. Ahmed S.K., J.-K. Peng, and D.J. Chmielewski, "Covariance-Based Hardware Selection-Part III: Distributed Parameters Systems" *AIChE J.*, 58(9), pp 2705-2713, (2012).

Refining Technology to Improve Feed Flexibility and Product Value

Friday, March 13, 2015 (Ballroom, **FrB1**)

Chair: *Paolo Palmas* (UOP/Honeywell)

2:15 PM (FrB1a) Shale Oil Processing Challenges: From the Reservoir to the Refinery

Carl E. Weaver (Baker Hughes Inc)

Refiners continue to look for ways to maximize profitability in their operations. The growing streams of shale oil, heavy crudes, and bitumen-based crudes entering refineries for processing present an opportunity to capitalize on profits, but also pose tremendous challenges along the entire value chain from the reservoir to the refinery. Increased wax deposition, corrosion, and fouling are a few of the repercussions associated with the influx of unconventional crudes. If the quality of the crude can be managed throughout the process, challenges can be met more effectively, and damages to assets can be minimized. Understanding the impacts on crude quality at every stage, and knowing how to test and treat at each phase helps preserve the integrity of assets, enhance profitability and ultimately returns on investment throughout the value chain.

2:35 PM (FrB1b) Turning a Tier 3 Profit

Jame Esteban (Criterion Catalysts and Technologies)

Currently refiners are seeking options to address reductions in gasoline pool sulfur as required by the US EPA in 2017 as part of the Tier 3 regulations. However, several customers working with Criterion have already made strides to both meet the future Tier 3 regulations and are reaping the benefits of early success.

With advantages in volume swell, hydrogen upgrade, and operating cost structure these refineries are turning a profit from the new stringent regulations. These profits have been realized as increases in gasoline volume from improved FCC feed quality and operations, distillate (specifically ULSD) volume via synergies in co-processing, as well as overall refining capacity improvements.

While profitability as it relates to Tier 3 upgrades are contingent on refinery configuration, this paper explores the options and solutions employed with case studies from Criterion's extensive portfolio demonstrating these benefits.

2:55 PM (FrB1c) Tailoring Hydrocarbon Product Properties – Simple Solutions, Challenges, Limits – How to Find the Right Tools

Rainer Rakoczy, Dieter Himsl (Clariant)

The field of industrial hydrocarbon products goes far beyond fuels and lubricants, and the potential applications are nearly limitless. It goes without saying with so many possible applications that a huge variety of product properties exist. How effective a product is can vary in relation to how the properties change, especially if it gets cold.

In automotive applications, lubricity agents need to retain a certain viscosity across a broad temperature window. Jet fuels must remain fluid even at very high aviation cruising levels. Diesel fuel needs to remain fluid and dispensable when exposed to arctic conditions. It is a major concern when these important fluids change their functionality and solidify. Temporary breakdowns are not the only consequences of changing cold flow properties; it can even accelerate wear of critical parts.

Hydrocarbon products are derived from natural carbonaceous sources such as coal, crude oil or natural gas. Unfortunately, key properties of intermediate cuts derived from these sources vary dramatically, and technical know-how is necessary to achieve the right applicable specifications for the final product. Clariant has a broad portfolio of catalytic solutions and expertise in tailoring properties of hydrocarbon products. The field of application ranges from smooth hydrotreating for adjusting optical appearance of base oils to de-aromatization of intermediate cuts to tailoring cold flow properties for achieving diesel fuel grades to withstand Arctic winters.

Together with clients and capable engineering partners an optimum technical solution to achieve desired product properties can be found. Beginning with critical feedstock analysis, followed by feasibility and complexity studies, and ending with technical realization, it is possible to help the client produce a high value product. In this contribution theoretical and realistic cases of tailoring hydrocarbon product properties are shown to provide an idea of simple solutions, challenges and even limits, especially facing changes in quality of the carbonaceous sources historically or geographically.

[1] R.A. Rakoczy, P.M. Morse, 'Consider catalytic dewaxing as a tool to improve diesel cold flow properties' in *Hydrocarbon Processing*, July 2013.

[2] E. O. Köhler, 'Catalytic dewaxing with zeolites for improved profitability of ULSD production' in *FROM ZEOLITES TO POROUS MOF MATERIALS – THE 40TH ANNIVERSARY OF INTERNATIONAL ZEOLITE CONFERENCE*, Ruren Xu, Zi Gao, Jiesheng Chen, Wenfu Yan, *Studies in surface science and catalysis* 170 B (2007) 1292, ELSEVIER.

3:15 PM (FrB1d) Innovative Process Changes for Improved LPG and Hydrogen Recovery in Platforming™

Robert Tsai, William Yanez, Frank (Xin X.) Zhu
(UOP/Honeywell)

The inclusion of a downstream vapor-liquid recontacting scheme within a catalytic reforming (PlatformingTM) process is a typical means to enhance recovery of hydrocarbons (C3+ material, but with traditional focus more on C5+ material) in the liquid phase and likewise improve hydrogen purity of the net vapor. Many recent design efforts have been made to increase both LPG (C3/C4) and hydrogen recoveries because of their value in current markets; if not recovered, these components are lost in the fuel gas as by-products. This presentation describes design solutions that are not only capable of achieving extremely high recoveries of these valuable products but can also be tuned based on specific customer targets.

A fairly conventional recontacting flowscheme is considered in this application. This configuration is capable of recovering LPG to a certain extent but possesses inherent inefficiencies that make achieving very high recoveries quite challenging. An improved design is covered, which enables recovery to be maximized without introducing much additional complexity versus the conventional recontacting scheme. A hybrid separation concept is also discussed, for cases where a pressure-swing adsorption unit (for further hydrogen purification) is located downstream of the recontacting section.

3:35 PM (FrB1e) **Refinery Forensics - Using Microscopy and Microanalysis in Refinery Trouble Shooting and Problem Solving**

Bradley Huggins (North Twin Microscopy Inc.)

Over approximately the past two decades, the science and technologies that are included in the areas of microscopy and microanalysis have continually evolved, greatly broadening the potential application of these techniques to Refinery and Petrochemical Processes. Among the major advances in these technology areas are some key instrumental advances, including: 1) the substantial development of environmental scanning electron microscopy (ESEM) and variable pressure SEM; 2) Advances in higher resolution, field emission-SEM instrumentation; 3) advances in x-ray microanalysis detection, using much more efficient silicon drift detectors and greatly improved x-ray microanalysis application software systems; 4) integration of light and electron microscopy with various optical spectroscopies; and 5) Advances in SEM electron beam optics and electron image detection modes and better control of the electron beam and specimen interaction.

Microscopy and microanalysis can now be more effectively applied to materials such as Refinery Process - scales, salts, sludges, and films, as well as other more typical and stable materials such as solid components, metals and metallurgy, catalysts, and other related materials. With this potential for more versatile and broader application, the benefits of microscopy and microanalysis can better contribute in the analytical characterization of Refinery and Petrochemical Processes. Fast and direct characterization of the inorganic components (and many organics) can be performed in the ESEM providing morphology and elemental analysis in a semi-

quantitative manner, and often with some ability to obtain some chemical information. This can enable a rather forensic approach to Refinery Process problem solving. When combined for example with FT-IR and other spectroscopic characterizations, a comprehensive analysis can include all components with identification of elements and phases, providing a detailed fingerprint of a problem material.

Catalysis for Chemicals Synthesis

Friday, March 13, 2015 (Armour Dinning, FrB2)

Chair: *Michael Caracotsios* (UOP/Honeywell)

2:15 PM (FrB2a) **Controlling Au Particle Sintering During the Hydrochlorination of Acetylene Using Core-Shell Bimetals**

Kerry C. O'Connell, John R. Monnier, John Regalbuto
(University of South Carolina)

Introduction: Polyvinyl chloride (PVC) is the third highest global volume plastic after polyethylene and polypropylene, and the demand increases annually. In 2008, the PVC world market reached a volume of 34 million tons, while PVC demand is expected to total more than 40 million tons in the year 2016 [1]. PVC is produced from polymerization of vinyl chloride monomer (VCM), which is typically produced industrially by the dehydrochlorination of dichloroethane (ethylene-based process) or hydrochlorination of acetylene (acetylene-based process). In commercial acetylene-based process, acetylene (C₂H₂) gas reacts with anhydrous hydrogen chloride (HCl) gas over carbon-supported mercuric chloride to produce VCM. This reaction is exothermic and highly selective at an optimum reaction temperature of about 170–180°C [3–5]. The major problem of this process is sublimation of mercury, arising from reduction of mercuric chloride during the reaction. Previous research groups have reported a direct correlation between the standard reduction potential of noble metals and acetylene conversion and concluded that gold is a potential catalyst to replace the mercuric based catalysts as the preferred catalyst for this reaction [4-5].

Electroless Deposition (ED) and Strong Electrostatic Adsorption (SEA) are used in conjunction in this study to for a rational synthesis methodology to produce highly dispersed Au mono and bimetallic catalysts with a core@shell morphology to reduce the sintering of Au nanoparticles during reaction by depositing gold selectively onto a metal with higher surface free energy.

Materials and Methods: 1% Au/C and Pt/C catalysts were prepared via SEA using Bis(ethylenediamine)gold(III) Chloride(Auben) or Tetraammineplatinum(II) chloride and Darco KBB activated carbon with a point of zero charge of 4 and a measured surface area of 1100 m²/g. To deposit Au on a well dispersed noble metal catalyst ED was used at room temperature using KAu(CN)₂ as the metal salt with hydrazine as the reducing agent at pH 9. Various coverages in theoretical monolayers were used to ensure full coverage of the core metal (i.e. Pt) and this was confirmed using pulse

chemisorption along via PXRD to confirm particle size pre and post reaction.

Acetylene hydrochlorination using the supported Au catalysts was carried out in a fixed bed glass reactor. The following reaction protocol was used for all catalysts. The reactor loaded with fresh catalyst was dried in flowing helium at 180° C for 30 min to remove residual water and then pre-chlorinated using a flow of He and HCl (1: 1 ratio) at ° for 1 h. Acetylene was then added at a desired flow to give a feed composition of C₂H₂: HCl: He = 1.0: 1.1: 1.0 at an initial reaction temperature of 180°C.

Results and Discussion: Au particle sintering occurs rapidly in the presence of HCl during both pretreatment and reaction. The stability of Au nanoparticles and the active species AuCl₃ is important in the long term activity of Acetylene hydrochlorination. 1% Au catalysts prepared via SEA at 1.5nm agglomerate to 20nm after just 5 min in 10ml/min HCl during pretreatment, there is not significant further growth after the rapid initial sintering.

The use of a core metal to anchor a gold shell onto is being studied as a way to limit particle agglomeration, as under similar conditions metals like Pt and Pd do not undergo particle growth while selectively depositing Au on a stable base metal seems promising for further study.

2:35 PM (FrB2b) Vapor phase Ethanol Carbonylation over Supported Rhodium Catalysts

Sara Yaco and Sunyong Park (Northwestern University), Beata Kiloa and David Barton (Dow Chemical), Justin Notestein (Northwestern University)

Results will be discussed for vapor phase ethanol carbonylation to propanoates over supported rhodium catalysts.

2:55 PM (FrB2c) Counting Active and Selective Sites on Niobia-Silica Catalysts for Alkene Epoxidation with H₂O₂

Nicholas Thornburg, Justin Notestein (Northwestern University)

We discuss the application of a selective organophosphonate catalyst poison for in situ titration of silica-supported Nb(V) oxide sites for quantifying intrinsic reactivity and selectivity in the epoxidation of alkenes with H₂O₂, as may be relevant for the production of important epoxy monomers.

3:15 PM (FrB2d) Ethylene Carbonylation by Molybdenum Carbonyl Catalysts

Chieh-Chao Yang (Northwestern University), Beata Kilos and David Barton (Dow Chemical), Eric Weitz and Justin Notestein (Northwestern University)

This talk will discuss ethylene carbonylation by molybdenum carbonyls, as relevant to the production of propanoates, which are important chemical intermediates.

3:35 PM (FrB2e) Effects of Solvent and Substituents on the Kinetics of Di-Olefin Epoxidation Catalyzed by Fe-porphyrin Complexes

Ying Yu, Linda J. Broadbelt (Northwestern University)

Epoxy resins are important industrial materials commonly used in paintings, coatings and electronic packaging. Novel epoxy resin formulations utilize certain types of di-epoxides, which are usually produced from di-olefins, to achieve better physical properties. Recently, a family of biomimetic catalysts, Fe-porphyrin complexes, has been discovered to have a wide range of catalytic reactivity and selectivity towards di-olefin double epoxidation with a clean oxidant, H₂O₂. However, the underlying mechanism accounting for performance of different Fe-porphyrins is not well understood.

In this study, we investigated the effects of solvent and substituents on the kinetics of epoxidation catalysis. Two solvent effects were addressed for methanol solvent: how methanol participates in epoxidation catalysis, and how methanol axial ligand influences the energetics. For substituent effect, fluorinated catalyst (Fe-por-F) and hydrogenated catalyst (Fe-por-H) were studied, as they have the highest and lowest selectivity towards epoxidation in experiments, respectively. All possible spin states were considered. We adopted the most general mechanism proposed in the literature to date [1] and focused on the two bifurcating rate-determining steps, heterolysis and homolysis, which lead to di-olefin epoxidation and H₂O₂ decomposition, respectively. Density functional theory (DFT) calculations were then conducted to elucidate the detailed mechanism of these two steps. Finally, microkinetic modeling was used to simulate the kinetics of the two competing reactions and to rationalize the selectivity.

DFT calculations were performed with the B3LYP functional using Gaussian 09. Two basis sets were employed: BS1 (LANL2DZ (Fe)/6-31G(d) (other atoms)) was used for geometry optimization, while a larger one, BS2 (LANL2TZ(f) (Fe)/6-311+G(2d,p) (other atoms)), was used for single-point energy evaluation with a polarizable continuum model (PCM). A microkinetic model was built for the two rate-determining steps in terms of elementary steps.

Quantum chemical calculations revealed the free energy profiles of the two competing rate-determining steps. Methanol was found to be an acid-base catalyst in heterolysis. Species without methanol axial ligand are much more favorable energetically, as methanol coordination significantly raised the free energies of transition states in both heterolysis and homolysis. Microkinetic modeling results showed significant substituent effect on the selectivity towards heterolysis. At the end of simulation, the selectivity to heterolysis is two orders of magnitude higher for Fe-por-F compared with Fe-por-H. Under the assumption that the final epoxide yield is directly influenced by the selectivity towards heterolysis, our computational prediction is in excellent accord with experimental results, in which Fe-por-H catalyst gives almost zero epoxide yield, while Fe-por-F has as high as 75% epoxide yield.

This study elucidated the detailed mechanism of Fe-porphyrin-catalyzed di-olefin epoxidation, and evaluated solvent and

substituent effects. Ultimately, this research provides a basis for the design of new biomimetic catalysts for di-olefin epoxidation.

[1]. Stephenson, N. A., Bell, A. T. *J Mol Catal a-Chem Appl.* 275, 54 (2007).

3:55 PM (FrB2f) Gas-Phase Dimerization of Ethylene under Mild Conditions Catalyzed by MOF Materials Containing Ni(II) Bipyridine Complexes

Sherzod T. Madrahimov, SonBinh T. Nguyen (Northwestern University)

A highly porous MOF material containing (bipy)NiII moieties was prepared through the solvent assisted ligand incorporation method. The obtained catalyst displayed catalytic activities that were comparable to those observed for highly active $(PPh_3)_2NiCl_2$ catalyst and up to an order of magnitude higher than the corresponding (bipy)NiCl₂ homogeneous system. Due to its high porosity the catalyst retained its outstanding levels of activity under mild conditions in the gas-phase ethylene dimerization reaction both under batch and continuous flow conditions.

Drug Delivery

Friday, March 13, 2015 (Alumni Lounge, **FrB3**)

Chair: *Georgia Papavasiliou* (Illinois Institute of Technology)

2:15 PM (FrB3a) A Controlled and Extended Drug Delivery System to Treat Posterior Segment Eye Diseases

Christian Osswald, Jennifer J. Kang-Mieler (Illinois Institute of Technology)

Current therapies for many posterior segment eye diseases require monthly or bimonthly bolus intravitreal injections of anti-vascular endothelial growth factors (anti-VEGFs). Less frequent administration via controlled and extended release of anti-VEGFs is needed to improve upon current therapies and lessen the potential side-effects and socioeconomic impact of repeat intravitreal injections. We have developed a drug delivery system (DDS) consisting of drug-loaded poly(lactic-co-glycolic acid) microspheres suspended within a thermoresponsive, injectable poly(N-isopropylacrylamide)-based hydrogel, which can be made to be fully biodegradable. Ranibizumab and aflibercept, two FDA-approved anti-VEGFs used to treat posterior segment eye diseases, were used to characterize the release and bioactivity of our DDS. Our DDS is capable of controlled release of both anti-VEGFs for approximately 200 days, with no toxicity observed in human umbilical vascular endothelial cell culture system at any time point. Release samples of both ranibizumab and aflibercept were able to inhibit VEGF-driven cell growth, suggesting that the anti-VEGFs remain bioactive. Initial in vivo results suggest that our DDS is non-toxic and that controlled and extended release of anti-VEGF provides a therapeutic advantage over bolus injection. The proposed DDS will greatly improve upon the current monthly/bimonthly anti-VEGF treatment regimens needed for many posterior segment diseases.

2:35 PM (FrB3b) Improved Induction of Apoptosis by Bortezomib loaded in Liposomal Nanocarriers: A Comparison between Cationic and Ceramide Liposomes
Medha Joshi, Gabriel Park, Jennifer Pichlik, Annette Gilchrist (Midwestern University)

Bortezomib (Velcade), a proteasome inhibitor, was encapsulated in two types of liposomal nanocarriers viz. cationic or ceramide in order to enhance its intracellular delivery and apoptosis induction. Cellular viability assay and apoptosis assay was conducted in related cell lines. By delivering bortezomib using liposomal nanocarriers cell death and apoptosis was increased in a time and dose dependent manner in comparison to bortezomib alone. Bortezomib is the standard of care for Multiple myeloma (MM). MM is a malignancy of terminally differentiated B-lymphocytes (plasma cells). The cancerous cells overwhelm the bone marrow and are associated with anemia and bone pain. Bortezomib, a proteasome inhibitor is capable of inducing myeloma cell apoptosis. However bortezomib must avoid lysosomal degradation while being delivered to its target, the proteasome located inside the cell to impart maximum efficacy. Targeted drug delivery to B cells using particulate drug carriers has been proven to be effective in the past to delivery their cargos inside the cell avoiding the lysosomal degradation. Increasing the dose efficacy of bortezomib by encapsulating in liposomes could also potentially reduce the side effects of bortezomib, such as peripheral neuropathy.

Two formulations of bortezomib encapsulated in liposomes, cationic (DOTAP) and ceramide, were developed. To investigate which formulation had better synergistic apoptotic effects, the changes in cellular metabolic activity were assessed on three different cell lines with the Alamar Blue assay. Cell death via the apoptotic pathway was assessed by flow cytometry. To better understand the consequences of bortezomib on bone cells, three different cell lines were tested; an osteoblast mouse calvaria cell line (MC3T3), a pre-osteoclast mouse cell line (RAW264.7), and an osteosarcoma human cell line (U2OS). Liposomes were prepared by dry film evaporation technique, characterized in terms of particle size, zeta potential, and loading efficiency. Both liposomal formulations were prepared multiple times and measured for particle size, polydispersity index, zeta potential and loading efficiency (HPLC). Treatment of these cell lines with cationic bortezomib liposomes resulted in significantly reduced metabolic activity in MC3T3 cells, RAW 264.7 cells, and U2OS cells compared to bortezomib alone at 24 h and 48 h, respectively (all $p < 0.01$). These results were quite distinct from ceramide bortezomib liposomes which were found to have higher pIC50 values compared to bortezomib alone at 24 and 48 h of exposure in all three cell lines, but only the pre-osteoclast cell line (RAW 264.7) were found to be statistically significant at both 24 h and 48 h ($p < 0.01$ and $p < 0.05$), respectively). In the apoptosis assay using fluorescent-activated cell sorting (FACS), on RAW cells pretreated with bortezomib alone and encapsulated in ceramide, the latter

resulted in higher number of cells undergoing apoptosis (lower right quadrant) at the 1 nM concentration ($p < 0.01$) and higher number of cells undergoing both cell death and apoptosis (upper right quadrant) at the 10 nM concentration ($p < 0.05$). Results indicate that encapsulation of bortezomib into ceramide or cationic liposomes may enhance its effects on osteoblast and osteosarcoma cells, and such an approach may provide a useful treatment for patients with osteosarcomas.

2:55 PM (FrB3c) **Engineering Exosomes as Therapeutic Delivery Vehicles**

Michelle E. Hung, Joshua N. Leonard (Northwestern University)

Exosomes are biological nanovesicles that transfer proteins and nucleic acids between cells and have great potential as tunable therapeutic delivery vehicles; they are relatively easy to engineer, well-tolerated in vivo, and naturally capable of intracellular delivery of functional biomolecules. In order for this promise to be realized, robust and general methods for incorporating therapeutic cargo molecules into exosomes and for targeting therapeutic exosomes to specific destinations in vivo are required.

Loading therapeutic RNA into exosomes poses several challenges. Transfer of RNA into isolated exosomes by electroporation can be inefficient and generates RNA precipitates. Alternatively, mass-action-driven incorporation, in which the therapeutic RNA is overexpressed in exosome producing cells, is attractive but has not been as widely explored. In particular, it is not known how native RNA sorting and processing mechanisms and biophysical limitations may impact the efficacy of this approach for different RNA cargo molecules. Thus, to provide a robust and orthogonal strategy for exosome loading, we have developed a Targeted And Modular Exosome Loading (TAMEL) platform for directing the loading of a specific RNAs into exosomes. The TAMEL system comprises a packaging protein and a cargo RNA. The packaging protein is an RNA binding protein targeted to exosomes via fusion to an exosome-enriched protein. The cargo RNA is an RNA molecule displaying an RNA motif that is specifically bound by the packaging protein. Using this system, we have packaged small and large RNAs into exosomes and characterized the relationship between RNA size and packaging into exosomes by mass action alone or targeted means. This platform enables us to package mRNAs and RNAi-inducing RNA species into exosomes and to quantitatively evaluate delivery and functional modulation of gene expression in recipient cells. To enhance delivery of therapeutic exosomes to target recipient cells, we have also developed a technology for enhancing the display of targeting ligands on the exterior of exosomes. Previous attempts to target exosomes to specific recipient cells have been hindered by inconsistent targeting using different ligands or different exosome-producing cell types. We determined that degradation of targeting peptides by endosomal proteases occurs during exosome biogenesis. To overcome this challenge, we have also developed a

glycosylation strategy that protects peptides from degradation while maintaining their ability to bind target proteins. We applied this peptide targeting strategy to engineer enhanced delivery of exosomes to prostate cancer cells. The tools we have developed enable programming exosomes for targeted delivery of RNA cargos in a robust and straightforward manner that can be applied to a wide variety of therapeutic targets.

3:15 PM (FrB3d) **“Shake-n-Incubate”: Examining the Effects of Orbital Shaking on Iron Oxide Nanoparticle Uptake for Stem Cell Labeling**

Nicholas E. Clay (University of Illinois Urbana-Champaign)

Labeling stem cells with superparamagnetic iron oxide nanoparticles (SPIONs) enables clinicians to assess the bioavailability and localization of transplanted cells through MR imaging. To facilitate the cellular uptake of SPIONs for cell therapies, previous labeling protocols optimized the concentration, size, surface charge, and targeting capability of SPIONs. However, these approaches have demonstrated only moderate degrees of success, as the MR signal from the cells falls in vivo due to SPION exocytosis or degradation. To improve SPION content per cell, we sought to control cell labeling by manipulating the cellular microenvironment while keeping the intrinsic properties and concentration of the nanoparticles constant. To this end, we prepared SPION clusters formed by the hydrophobic association between SPIONs and poly(2-hydroxyethyl aspartamide) substituted with hydrophobic octadecyl chains. These water-stable, monodisperse SPION clusters have a T2 relaxivity comparable to Feridex, an FDA-approved MR contrast agent. We incubated bone marrow-derived mesenchymal stem cells in cell culture media suspended with SPION clusters while shaking the cell culture well at varying rates. Cells exposed to orbital shaking at 50 rpm took up more SPIONs than cells cultured in static culture wells, as quantified through ICP. In addition, cells cultured under shaking at 50 rpm exhibited a lower T2 signal than those cultured without any external mechanical flow. Interestingly, the role of orbital shaking on SPION uptake was insignificant when serum concentration in the cell culture media was decreased. This intriguing protocol will be extended to label a wide array of therapeutic cells, in turn improving transplanted cell tracking and, ultimately, the success of cell therapies.

3:35 PM (FrB3e) **Controlled Vancomycin Release from a Biodegradable Hydrogel Ocular Drug Delivery System**

Emily Dosmar, Jennifer J. Kang-Mieler (Illinois Institute of Technology)

This study investigated potential use of an injectable, biodegradable hydrogel that delivers prophylactic vancomycin (VAN) for two weeks following ocular surgery to replace conventional topical eye drop treatment. The goal is to deliver a controlled and sustained delivery of VAN for duration of 2 weeks as well as eliminate topical treatment to avoid chronically low patient compliance. The proposed drug delivery

system consists of VAN encapsulated in hydrolytically degradable poly(ethylene glycol)-co-(L-lactic acid) diacrylate (PEG-PLLA-DA) and poly(ethylene glycol) diacrylate (PEG-DA) hydrogels. Hydrogel characteristics of the system including degradation time, swelling ratio, mesh size, and release were investigated. Hydrogel swelling ratios decreased with increased PEG-DA concentrations. Hydrogel mesh size was estimated to be 6.79-7.76 nm regardless of investigated polymer composition. Complete degradation ranged from 3-16 days and hydrogels degraded more slowly as polymer concentration increased. Hydrogels with a higher degradable to non-degradable polymer ratio showed a faster overall degradation time and hydrogels with the same polymer ratio degraded more quickly with lower PEG-DA molecular weight. VAN release from hydrogels occurred over two weeks with ~30% release of theoretically encapsulated VAN in the first 24 hours. Overall, these hydrogels show promise for application as prophylactic ocular drug delivery devices.

3:55 PM (FrB3f) Sustained Delivery of a VEGF Mimetic Peptide for Scaffold Neovascularization

Daniel A. Young, Georgia Papavasiliou (Illinois Institute of Technology)

Sustained delivery of neovascularization factors has been shown to lead to mature vessel formation in tissue engineered scaffolds. While growth factors are commonly used to promote angiogenic cell behavior, they are costly to manufacture and susceptible to degradation. A promising alternative is peptide sequences designed to interact with specific receptors, namely those which growth factors use to regulate neovascularization pathways for stimulating vessel formation in scaffolds. We have developed a synthetic poly(ethylene glycol), PEG, hydrogel nanoparticle carrier system that allows for tunable release kinetics of angiogenic peptides through alterations in nanoparticle (NP) crosslink density and hydrolytic degradation rate. Sustained release of a vascular endothelial growth factor-mimetic peptide, QK, was achieved in NPs of varying crosslink density/diffusivity and degradation. Data indicate that increases in the crosslink density of non-degradable NP carriers results in increases in the duration of release, with a cumulative release of 10 µg QK per mg NP at 2 weeks or 6 weeks for the high and low crosslink density NPs, respectively. Rendering the NP crosslinks hydrolytically degradable while maintaining their initial crosslink density resulted in a higher level of peptide to be released (50 µg QK per mg NP at 2 weeks). NPs were characterized in terms of particle size distribution using nanoparticle tracking analysis (155.0 ± 77.9 nm), surface charge (zeta potential of -29.6 ± 5.84 mV), and crosslink density by gravimetric swelling ratio measurements (inversely related to crosslink density, 17.2 ± 5.0). Current studies are aimed at investigating the role of QK release kinetics on scaffold neovascularization in vitro.

Power and Energy Systems

Friday, March 13, 2015 (Crown Room, **FrB4**)

Chair: *William Ryan* (University of Illinois at Chicago)

2:15 PM (FrB4a) Promise Kept

Richard Meyer (American Gas Association)

The past five years have seen an unprecedented rise in unconventional natural gas production from shale formations, prompting many to recognize the promise of sustained and affordable natural gas resources for years to come. More recently the polar vortex across the US prompted unprecedented requirements of natural gas as demand soared to all-time records. This presentation will examine recent changes in natural gas markets, acknowledging industry performance during the past two winters (2013-2014, and 2014-2015). Topics include factors related to record production and new demand, and a look at growth possibilities including how policy may affect prospects for natural gas markets in the years ahead.

2:35 PM (FrB4b) Generation IV Sodium Cooled Fast Breeder Reactors

Emmilyn Riley (University of Illinois at Chicago)

Most of the reactors in use today are called thermal reactors, in which neutrons born from fission are slowed down by a moderator to cause new fissions. The focus of this paper is another type of reactors, called fast neutron reactors, or simply fast reactors. The paper explores fast reactors that are cooled by liquid sodium and allowed to operate in a breeder configuration to produce more fuel than they consume. These reactors are called sodium cooled fast breeder reactors, or SFRs. Advantages of and challenges faced by SFRs will be extensively compared.

2:55 PM (FrB4c) Solid Oxide Fuel Cells for Energy Production, Conversion and Storage

Rick Dombrowski (University of Illinois at Chicago)

Fluctuating electric demand challenge the grid in providing reliable electricity. Renewable energy has recently been incorporated onto the grid, but is handcuffed to the forces of nature. Currently there are few ways to efficiency store electricity or produce on-demand renewable electricity. Solid-oxide fuel cells (SOFCs) are a type a fuel cell that operate at high temperatures and can use hydrocarbons as fuel. This allows SOFCs to easily be integrated with existing technologies for energy production. SOFCs can also operate as a Solid Oxide Electrolysis Cell. As a result, electricity from renewable energy that is produced during periods of low-demand can be converted and stored as a fuel for use at a later time. The advancements in SOFC technology has led to several designs that may soon allow the technology to break into the energy market.

3:15 PM (FrB4d) Movable Bulb Turbine for Low Head Hydropower

Nikolay Popov (University of Illinois at Chicago)

We are going to explore and evaluate the latest technological developments in Hydropower, as well as the opportunities for real world applications. Research suggests that there is still a vast untapped resource in harnessing the power of low head rivers. Therefore, the focus of the paper will be the very recent developments in low head Hydropower. Aside from the technological characteristics, we will look into the regulatory policies and financial aspects including investment costs, operation and maintenance costs. Finally, we will review the environmental impact of this technology and compare it with other power generation options.

3:35 PM (FrB4e) **Business Model of Leasing Photovoltaic Solar Systems**

Aidan Gilbert (University of Illinois at Chicago)

Third party ownership of solar panel systems has brought upon a great deal of growth in the solar market. Through third party ownership, companies establish lease agreements with homeowners to install and maintain a solar panel system where the homeowner makes monthly payments for the system, but still has a lower bill than before the installation. This business model is based around governmental policies that give tax incentives to the leasing companies and their investors. This paper will explore the role of the four agents involved in a solar lease: the homeowner, the leasing company, the investors and the local utility. The model of solar leasing companies varies between different companies and continues to evolve as market the changes. This paper will also discuss the debate between third party ownership and direct ownership and how the consumer would weigh the pros and cons of each option. Additional challenges for the different agents of the lease will be addressed as well. Lastly, there will be a brief outlook on the solar leasing market for the future as the market continues to evolve.

3:55 PM **Multiphase CFD and its application in precombustion CO₂ capture processes** (FrB4f)

Emad Ghadirian Hoseinabadi, Shahin Zarghami, Hamid Arastoopour, Javad Abbasian (Illinois Institute of Technology)

Climate change caused as a result of increase in the concentration of CO₂ in the atmosphere is one of the major challenges of 21st century. One of the most promising approaches to Carbon Capture and Storage (CCS) is to use solid sorbents and the fluidized bed process in pre-combustion IGCC plants, however this process currently is not ready for implementation in coal-based power plants. One of the major challenges, hindering its application, is the fact that it is still in the lab or bench scale stages. To successfully scale-up such processes, a powerful tool, like Computational Fluid Dynamics (CFD), is needed. In this presentation numerical simulation of the CCS process in a 3D Fluidized Bed (FB) at 500 °C and 50 atm for the regeneration of MgO-based sorbents will be presented using an Energy Minimization Multi-Scale (EMMS) approach calculating momentum transfer between phases. EMMS is used

for capturing heterogeneities in the bed and the interactions between structures with different sizes and formation of clusters, which leads to inhomogeneity in the system, and calculating drag between phases. Constitutive equations based on Kinetic Theory of Granular Flow (KTGF) to represent hydrodynamic behavior of this system and a Shrinking Core Model (CSM) to represent the regeneration reaction are used.

Advances in Optimization II

Friday, March 13, 2015 (Herman Lounge, **FrB5**)

Chair: *Fouad Teymour* (Illinois Institute of Technology)

Co-Chair: *Mustafa Cagdas Ozturk* (Illinois Institute of Technology)

2:15 PM (FrB5a) **Optimal Sensor Placement under Uncertainty in Water Network System with Better Optimization of Non-Linear Uncertain Systems (BONUS) Algorithm**

Rajib Mukherjee, Urmila M. Diwekar (Vishwamitra Research Institute)

Waters in cities and metropolitan areas are distributed through large networks comprising nodes and pipes. Due to recent threat in security, the water networks are found to be probable targets. It is therefore essential to secure distributed water networks and a probable way to do so is through the application of sensor networks. Sensors can be used to detect possible attack through timely detection of presence of contaminants. For that purpose it is essential to locate sensors in suitable positions that can minimize the effect of an attack. Due to the cost constrains, the number of sensors that can be used are limited. Thus, it is essential to locate the sensors optimally for minimum effect. The impact of an attack in water network system can be assessed with various ways including the number of people affected or the length of the pipes that is contaminated. Our objective is to minimize the number of affected people. There are various uncertainties present in the system. The demand of water at the nodes can be uncertain or the location of attack in the network and doses of contaminant can also be uncertain. The demand uncertainty will lead to the variation in flow pattern and the uncertainty in location and concentration of contaminant will lead to various concentrations of contaminants at different nodes in the network. With these uncertainties, the net impact also varies accordingly. In our research, we have incorporated these uncertainties to make the optimal sensor placement more robust.

In the present work we have used model network from EPANET to simulate the system's steady state behavior for different base cases. Due to the delay in information processing from the sensor, the demand uncertainty will have a normal distribution. This is analyzed using a technique from information theory to determine the most cost-effective network of on-line sensors by formulating a nonlinear, stochastic binary integer problem. Generally a stochastic non-linear programming method calculates the probabilistic objective function by repeated evaluation for each sample at every iteration. In BONUS, the

reweighting approach is used instead of repeated function simulation. This makes our method robust as well as efficient. The results show the importance of uncertainty consideration in water network and highlight the advantages of the BONUS algorithm in sensor network problem.

2:35 PM (FrB5b) **Controller Performance Assessment for Artificial Pancreas**

Jianyuan Feng, Kamuran Turksoy, Ali Cinar (Illinois Institute of Technology)

Artificial pancreas (AP) control systems can regulate blood glucose concentration in patients with type 1 diabetes using glucose concentration information from a continuous glucose monitor (CGM) to suggest appropriate insulin infusion rates [1]. We have already developed an AP control system based on generalized predictive controller and adaptive constrained weighted recursive identification methods [1, 2, 3]. However, the performance of control system may change due to large dynamic changes in human body, sensor faults and time-varying time delays. A controller performance assessment module is developed to evaluate the performance of the controller and initiate controller retuning if there is significant performance deterioration. The module consists of several controller performance indexes that capture different aspects of controller performance, which can be analyzed to detect if performance deterioration caused by any specific part of the controller. Then “faults” diagnosed by indexes are used for controller retuning.

Controller performance assessment module use information such as CGM reading, CGM prediction, insulin suggestion, insulin constrains and objective function in controller to generate controller performance indexes. As a result, 5 indexes are developed respectively to indicate model prediction error, model prediction error elimination speed, limitation of insulin constraints, weight distribution in objective function and dangerous region (hypoglycemia or hyperglycemia) potential. The performance of the module is illustrated with three controller faults, model prediction error, insulin constrains error, and weight ratio error. Controller parameters such as forgetting factor, model prediction, insulin constraints and weights in objective function are retuned accordingly. 30 subjects in the UVA/Padova metabolic simulator [4] are used in simulations to test the controller performance assessment module. The result indicate that controller with the proposed controller performance assessment module has a safer blood glucose concentration range, better model accuracy and more reasonable insulin suggestions than a controller without any retuning.

[1]. Turksoy, K., Cinar, A. Adaptive Control of Artificial Pancreas Systems- A Review. *Journal of Health care Engineering* vol. 5, no. 1, pp. 1-22, April. 2014.

[2]. Turksoy, K., Quinn, L., Littlejohn, E., Cinar, A. An Integrated Multivariable Artificial Pancreas Control System. *Journal of Diabetes Science and Technology* vol. 8, no. 3, pp. 498-507, April. 2014.

[3]. Turksoy, K., Quinn, L., Littlejohn, E., Cinar, A. Multivariable Adaptive Identification and Control for Artificial Pancreas Systems. *IEEE Transaction on Biomedical Engineering*, vol. 61, no. 3, pp. 883-891, March. 2014.

[4]. B. P. Kovatchev, M. Breton, C. D. Man, and C. Cobelli, “In silico preclinical trials: A proof of concept in closed-loop control of type 1 diabetes,” *J. Diabetes Sci. Technol.*, vol. 3, no. 1, pp. 44–55, Jan. 2009.

2:55 PM (FrB5c) **Optimization of Air Usage in Activated Sludge Processes**

Mustafa Cagdas Ozturk, Fernando Martin Serrat, Fouad Teymour (Illinois Institute of Technology)

Wastewater treatment plants are known to utilize excessive amounts of air in activated sludge tanks in order to maintain sufficient growth of biomass and proper mixing. This approach requires intensive usage of energy for the compression of air, and this comprises up to 60% of the energy burden of an entire wastewater treatment plant [1, 3]. Usually, the rate of aeration is kept high in activated sludge tanks so as to minimize the effects of abrupt changes in influent conditions, such as composition, temperature or volume [2].

In the present study, an advanced activated sludge tank model is employed to assess the feasibility of using decreased aeration rates with different profiles. The activated sludge tank model is a discretized dynamic PFR model, which was calibrated and validated with the historical data from the Stickney Water Reclamation Plant in Illinois. Consisting of a train 48 CSTR tanks, the discretized model allows individual manipulation of airflow rates at each CSTR, and is an expedient conduit for performing optimization and process control studies.

In order to investigate the ideal aeration profile, a mixed-integer nonlinear programming (MINLP) problem was devised using the model with the objective of maintaining at least 8.5 mg/L of dissolved oxygen and less than 0.1 mg/L of ammonia in the effluent. This was mainly done by choosing a number of pivot CSTRs along the entire activated sludge tank. Aeration rates in the pivot CSTRs were designated as optimization variables, and the aeration rates of the remaining CSTRs were calculated by linear interpolation using the neighboring pivot CSTR tanks. This allows for the utilization of different aeration profiles at different portions of the activated sludge tank. Open-loop simulations with the optimized aeration profiles obtained from this strategy have shown that the total rate of aeration can be reduced by up to 70% while maintaining the nominal effluent quality. Furthermore, optimized aeration profiles were tested dynamically with storm simulations. Finally, simplified versions of optimized profiles were calculated for preliminary implementations and tested against major storm events.

[1]. Daw, J., Hallett, K., DeWolfe, J., Venner, I., 2012. Energy Efficiency Strategies for Municipal Wastewater Treatment Facilities. National Renewable Energy Laboratory, Technical Report NREL/TP-7A30-53341.

- [2]. Owen, W.F., 1982. Energy in wastewater treatment. Prentice-Hall, Inc., Englewood Cliffs, NJ.
- [3]. Spellman, F., 2008. Handbook of water and wastewater treatment plant operations. CRC Press.

3:15 PM (FrB5d) **Optimization Framework for MINLP Problems with Pyomo: Applications in Infectious Disease Parameter Estimation**

Jianfeng Liu, Carl D. Laird (Purdue University)

The Pyomo modeling package is well suitable to construct meta-algorithms, since it provides a convenient and flexible framework with access to many optimization solvers and a large number of python libraries. In this work, we focus on the development of a tailored optimization strategy for the solution of Mixed-Integer Nonlinear Programming (MINLP) problems. The solution technique proposed here, as an extension of Outer Approximation (OA) algorithm, is an algorithm depending on iteratively solving a sequence of lower and upper bounding problems. With the help of Pyomo's built-in functions, the nonlinear terms in original MINLPs can be easily relaxed by a number of piecewise linear under- and over-estimators giving convex relaxations formulated as Mixed-Integer Linear Programming (MILP) problems. In addition, typical bound tightening strategies, such as optimality-based bound tightening (OBBT) and feasibility-based bound tightening (FBBT) are implemented. To show its application, our tailored optimization framework is used to solve infectious disease parameter estimation problems formulated as non-convex MINLPs.

3:35 PM (FrB5e) **Selecting Optimum and Ideal Energized Fluids for Natural Gas Fracking**

Urmila Diwekar (Vishwamitra Research Institute)

Hydraulic fracturing is the process of creating small cracks, or fractures, in underground shale formations to allow oil and natural gas to flow into the wellbore and thereby increase production. To fracture the formation, special fracturing fluids

are injected down the well bore and into the formation under high pressure. These fluids typically consist of approximately 90% water, 9.5% sand, and 0.5% chemicals. The volume of fluids used for this purpose depends upon a variety of factors, including the well type and the formation depth and geologic composition. For example, horizontal wells require more water than vertical or directional wells (because of the length of the borehole that will be fracture stimulated), and deeper shale formations require more water than shallower formations. In short, hydraulic fracturing is a water intensive activity and water disposal is a major problem. Furthermore, in some wells water is not an ideal fluid for fracking.

In this paper, we present a new approach in developing alternatives to water-based fracking fluids. Numerous authors have presented benefits of energized fluids for fracking. Recently, Sharma and co-workers presented a modeling approach for selecting energized fracking fluid for a particular reservoir. Several reservoir parameters are critical for fluid selection and there are number of objectives involved in selecting a particular fluid. Our goal is to find ideal fluid / combination of fluids to meet the reservoir parameters which are cost effective and environmentally benign thus reducing water usage for fracking.

In this work, we propose an interval analysis approach for finding optimal and ideal energized fluids for various wells. We will couple interval analysis with the fracking simulator to derive intervals for different properties of ideal fracking fluid for a particular well based on intervals for the various objectives. Once the property ranges are identified we will then search property databases like SYNAPSE and/or NIST to find these fluids with the ideal properties. It is possible that we will have to blend number of different compounds to get the optimal fluid and/or involve computer aided molecular design (CAMD) to find new chemical fluid which can satisfy the property and performance requirements.

AIChE Midwest Regional Conference

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AIChE Midwest Regional Conference High School Outreach Program

The high school outreach program occurs in parallel with the technical program and is intended to expose students to the engineering profession with a focus on the discipline of chemical engineering. The two programs overlap during the lunch hour, where HS student will have an opportunity to talk with engineering professions about work life and career path experience /advice. Students are expected to come away with an understanding of what engineers do and how they impact our lives daily. Guidance on how to prepare for a career in engineering will also be provided. The HS Outreach portion of the program is organized by the [Chicago Local Section of the AIChE](#) in partnership with the [Chicago Council on Science & Technology](#) and hosted by the [Armour College of Engineering](#) at the [Illinois Institute of Technology](#). There is no cost for students or teachers to attend, but preregistration is required. Contact Information: Ellen Kloppenborg (HS outreach committee chair) Ellen.Kloppenborg@Honeywell.com
Ross Ludwig (Pre-Collegiate Outreach, IIT) rludwig1@iit.edu

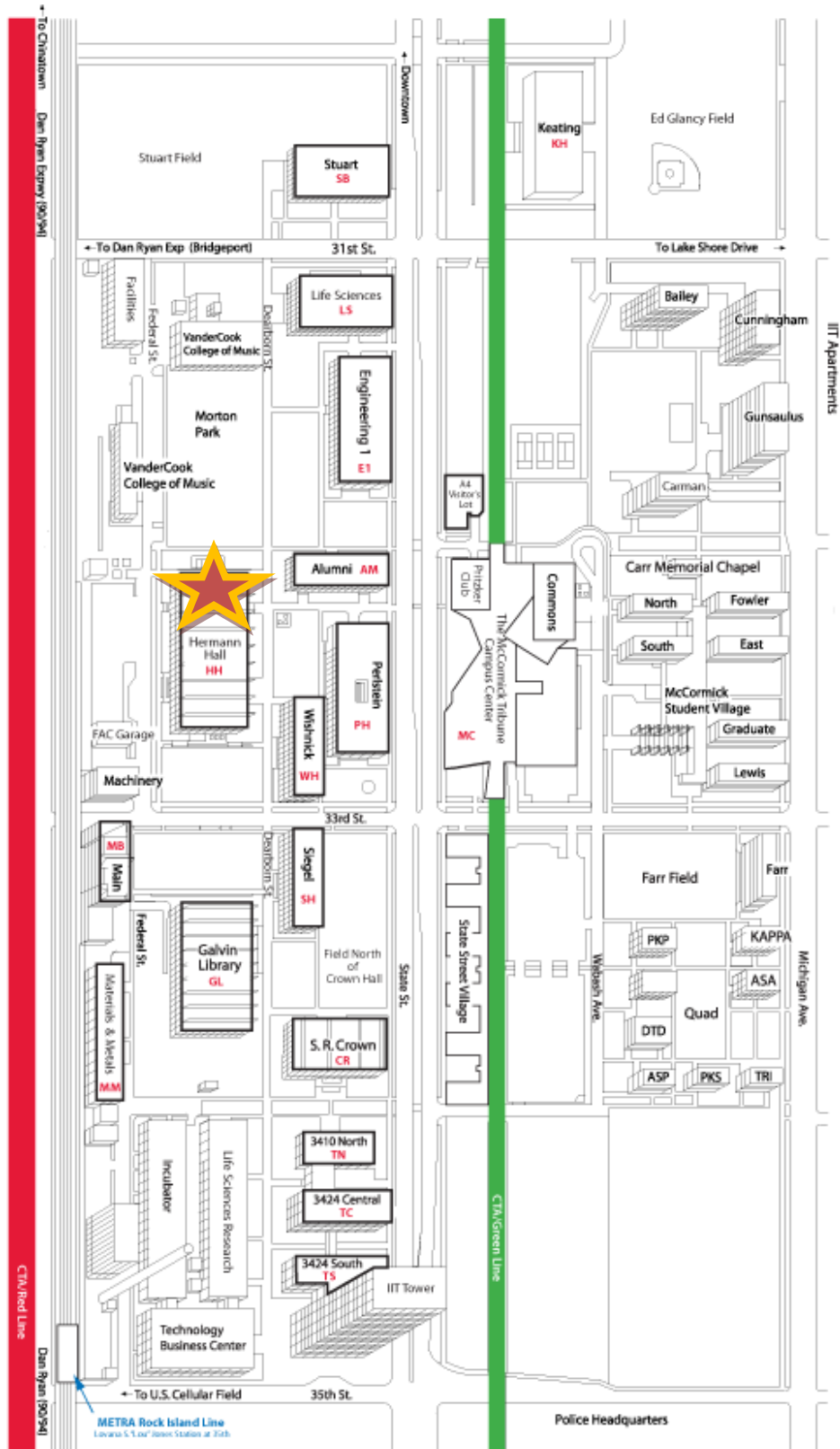
Time	Thursday, March 12, 2015	Friday, March 13, 2015
8:30 - 9:15am	Engineering Student Activities Fair - Meet with current engineering student organizations such as AIChE, SWE, NSBE, EWB and SHPE	Engineering Student Activities Fair - Meet with current engineering student organizations such as AIChE, SWE, NSBE, EWB and SHPE
9:15 - 10:00am	Presentation on Engineering Careers - Learn about how engineers contribute to all aspects of society	Presentation on Engineering Careers - Learn about how engineers contribute to all aspects of society
10:00 – 10:45pm	Demonstration Sessions - Robotics Demonstration, Formula Hybrid Race Car, Engineering Game	Demonstration Sessions - Robotics Demonstration, Formula Hybrid Race Car, Engineering Game
10:45 - 11:30pm	Engineering Panel Session - Learn about the day-to-day activities of practicing engineers and engineering students. Time to ask your most burning questions.	Engineering Panel Session - Learn about the day-to-day activities of practicing engineers and engineering students. Time to ask your most burning questions.
11:30 - 12:30pm	Engineering Lunch - Opportunity for one-on-one discussions with engineering professionals and students.	Engineering Lunch - Opportunity for one-on-one discussions with engineering professionals and students.
12:30 - 1:30pm	Keynote Speaker - Astronaut Al Sacco: first chemical engineer in space	Keynote Speaker - Astronaut Al Sacco: first chemical engineer in space
1:30 – 2:30pm	Tours of the IIT Campus	Tours of the IIT Campus

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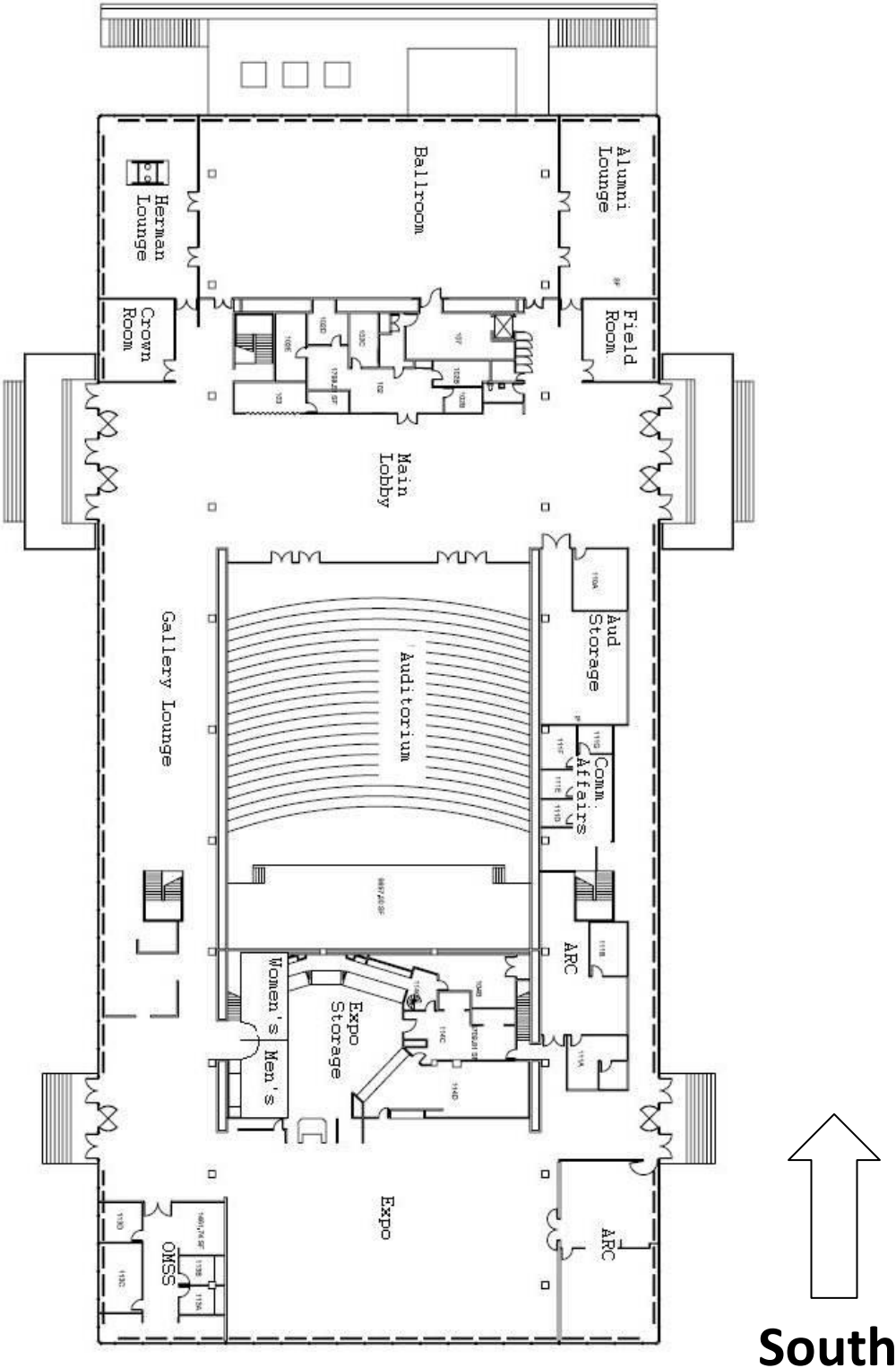
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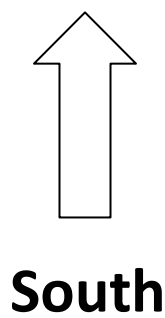
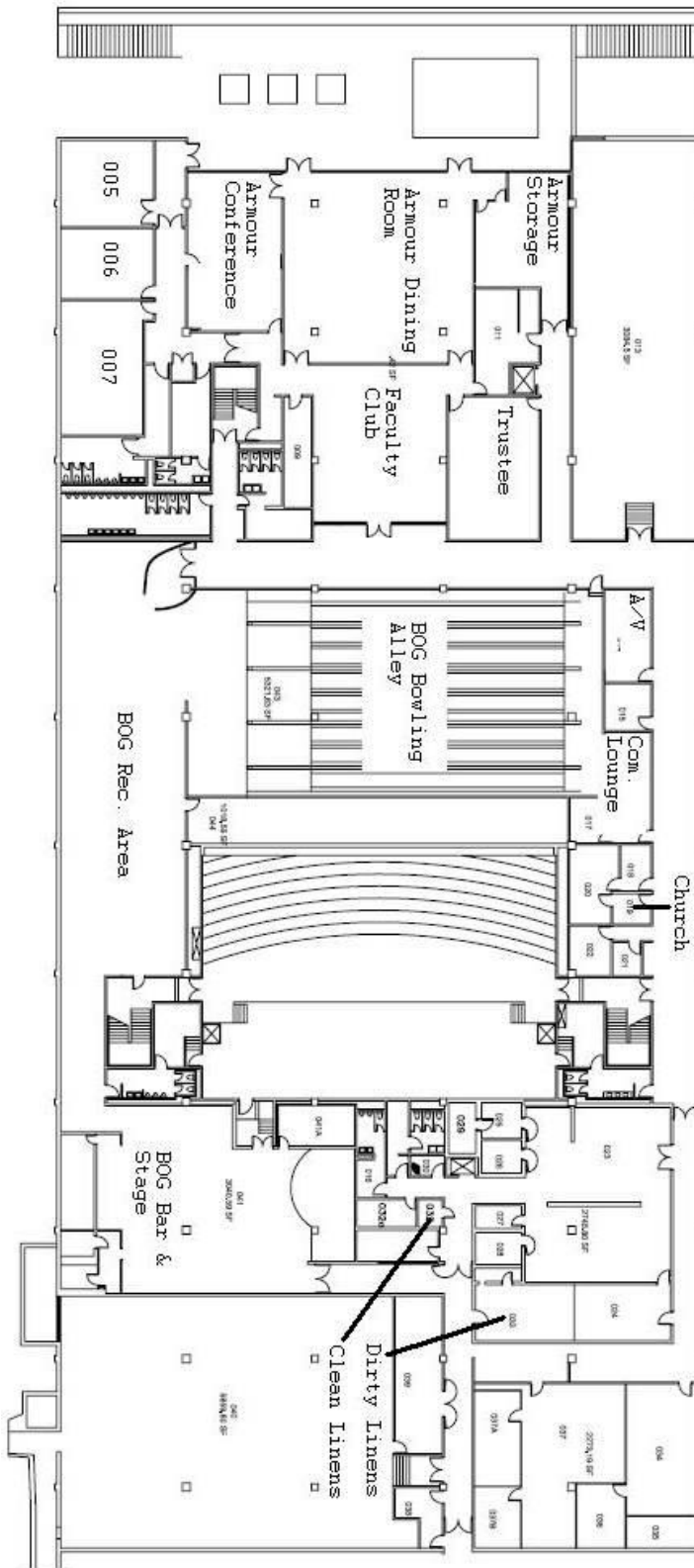
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Map of Herman Hall (first floor)



Map of Herman Hall (basement floor)



MRC 2016

8th Annual AIChE Midwest Regional Conference



Chicago - Spring 2016

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AIChE Midwest Regional Conference
Young Professionals Networking Social



What: YP Social after the 7th Annual Midwest Regional Conference at IIT

When: Friday, March 13th 5:30 – 8:30 PM

Where: Rocky's Chicago

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Soft drinks and appetizers provided courtesy of our
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