8TH ANNUAL

AIChE® MIDWEST REGIONAL CONFERENCE

March 3-4, 2016

Illinois Institute of Technology

· PROCESS SAFETY · REFINING · BIO-PROCESSING ·

· ENERGY · PROFESSIONAL DEVELOPMENT ·

Presented by the AIChE Chicago Section

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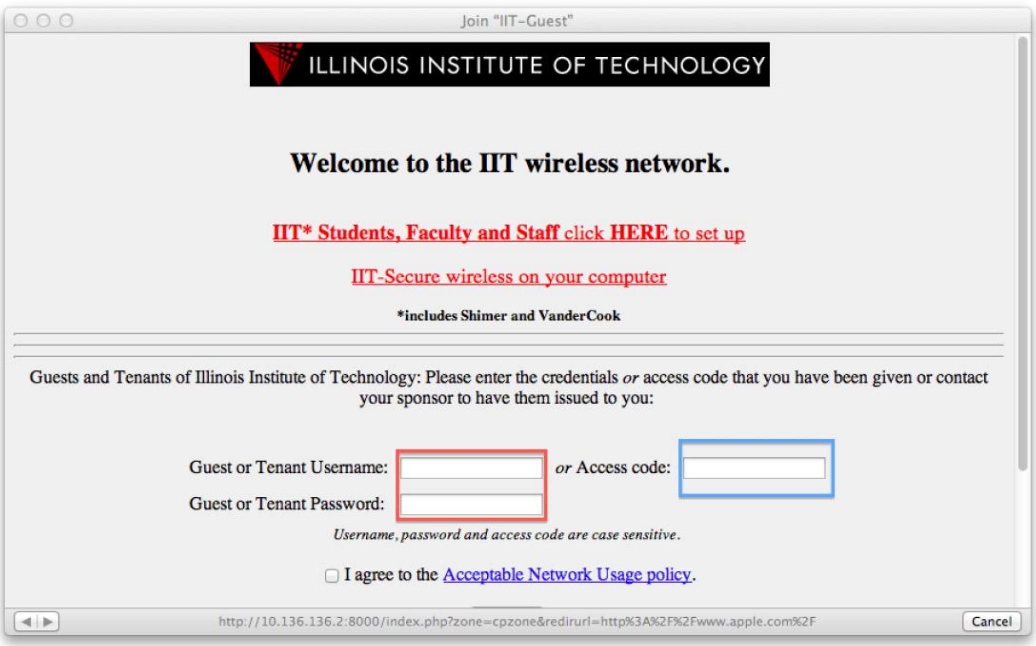

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 8th year. Organized by the **AIChE 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 **5 Keynote Lectures**: *Carlo Segre* (Illinois Institute of Technology), *Corey Correnti* (BP) and *Manu Vora* (Business Excellence, Inc.), **5 Plenary Lectures**: *Shakeel Kadri* (AIChE Center for Chemical Process Safety), *Linda Broadbelt* (Northwestern University), *Christopher Burcham* (Eli Lilly and Company), *Lorenz T. Biegler* (Carnegie Mellon University) and *Henrik Rasmussen* (Haldor Topsoe). There are **30 technical sessions** featuring over **140 oral presentations** over the 2 days of the conference.

The Thursday evening program is combined with the ***AIChE Chicago Local Section Monthly Meeting***. The meeting begins with a **Poster Session** and concludes with the **Dinner Keynote Lecture** by *Jeffery Hubbell* (University of Chicago).

The conference also features a **Student Outreach Program**, where Chicago-area high school students will become acquainted with the various facets of the chemical engineering profession. The outreach program features *Peter Ludovice* (Georgia Institute of Technology) as keynote speaker and includes a special luncheon where students can interact with practicing chemical engineers.

For young professionals, we have introduced two new **Professional Development Workshops**; one on *Chemical Process Safety* and second on *Leadership Excellence*. 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 8th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Patrick Shannon
Conference Chair
Middough Inc.

AIChE Midwest Regional Conference

Program at a Glance

Thursday, March 3, 2016

7:30 AM - 10:00 AM	**Continental Breakfast** (Gallery Lounge)
8:15 AM – 9:30 AM	**Morning Keynote** (Ballroom) - *Carlo Segre*, Professor of Physics, Illinois Institute of Technology
9:30 AM – 9:45 AM	**Networking Break**
9:45 AM – 11:30 AM	**Technical Sessions** - *Biofuels I* (Ballroom) - *Cancer Therapies* (Armour Dining) - *Process Safety I* (Alumni Lounge) - *Electro-Chemical Processes I* (Herman Lounge) - *Process Design and Optimization I* (Crown Room)
11:30 AM – 12:30 PM	**Lunch with High School Outreach Participants** (Ballroom and Expo Room)
12:45 PM – 1:45 PM	**Afternoon Plenary Sessions** - *Linda Broadbelt,* Professor and Chair, Northwestern University (Ballroom) - *Shakeel Kadri,* Executive Director, AIChE Center for Chemical Process Safety (Armour Dining)
1:45 PM – 2:00 PM	**Networking Break**
2:00 PM – 3:45 PM	**Technical Sessions** - *Biofuels II* (Ballroom) - *Drug Delivery I* (Armour Dining) - *Process Safety II* (Alumni Lounge) - *Electro-Chemical Processes II* (Herman Lounge) - *Multiphase CFD Tutorial* (Crown Room)
3:45 PM – 4:00 PM	**Networking Break**
4:00 PM – 5:45 PM	**Technical Sessions** - *The Hydrogen Economy* (Ballroom) - *Drug Delivery II* (Armour Dining) - *Process Safety III* (Alumni Lounge) - *Process Design and Optimization II* (Herman Lounge) - *Job Search Strategies* (Armour Conference Room)
5:45 PM – 6:30 PM	**Poster Session** (Gallery Lounge)
6:30 PM – 7:30 PM	**AIChE Chicago March Dinner Meeting** (Ballroom)
7:30 PM – 8:30 PM	**Dinner Keynote** (Ballroom) - *Jeffery Hubbell,* Institute for Molecular Engineering, University of Chicago

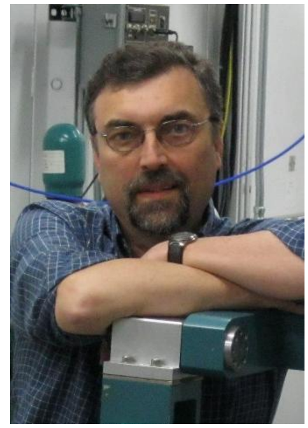
AIChE Midwest Regional Conference

Program at a Glance

Friday, March 4, 2016

7:30 AM - 10:00 AM	**Continental Breakfast** (Gallery Lounge)
8:15 AM – 9:30 AM	**Morning Keynote** (Ballroom) - *Corey Correnti,* Senior Vice-President, BP (retired, 2015)
9:30 AM – 9:45 AM	**Networking Break**
9:45 AM – 11:30 AM	**Technical Sessions** - *Process Modeling and Estimation* (Ballroom) - *Tissue Engineering I* (Armour Dining) - *Refining and Petrochemical Engineering I* (Alumni Lounge) - *Environmental Engineering* (Herman Lounge) - *Fluid Properties and Transport Phenomena* (Crown Room)
11:30 AM – 12:30 PM	**Lunch with High School Outreach Participants** (Ballroom and Expo Room)
12:45 PM – 1:45 PM	**Afternoon Plenary Sessions** - *Lorenz T. Biegler,* Professor and Head, Carnegie Mellon University (Ballroom) - *Christopher Burcham,* Senior Engineering Research Advisor, Eli Lilly and Company (Armour Dining)
1:45 PM – 2:00 PM	**Networking Break**
2:00 PM – 3:45 PM	**Technical Sessions** - *Process Operations and Control* (Ballroom) - *Tissue Engineering II* (Armour Dining) - *Refining and Petrochemical Engineering II* (Alumni Lounge) - *Pharmaceutical Processing* (Herman Lounge) - ~~*Process Safety Workshop I*~~ (Canceled) - *Leadership Workshop* (Armour Conference Room)
3:45 PM – 4:00 PM	**Networking Break**
4:00 PM – 5:45 PM	**Technical Sessions** - *Sustainable Power Systems* (Ballroom) - *Modeling of Biological Systems and Pathways* (Armour Dining) - *CFD Methods and Applications* (Alumni Lounge) - *Environmentally Conscious Process Design* (Herman Lounge) - ~~*Process Safety Workshop II*~~ (Canceled)
5:45 PM – 7:00 PM	**Closing Keynote and Reception** (Ballroom) - *Manu Vora,* President, Business Excellence, Inc. (Closing Reception Sponsor, *Baker Engineering and Risk Consultants*)
7:00 PM – 9:00 PM	**Young Professional Networking Social** (Off-Site) (YP Networking Social Sponsor, *Reactor Resourses*)

AIChE Midwest Regional Conference
Keynote and Plenary Speakers



Thursday Morning Keynote: 8:15 AM Thursday, March 3, 2016

Carlo Segre, Illinois Institute of Technology

Presentation Title: ***High Energy Density Nanoelectrofuel Flow Batteries for Transportation and Renewables: Development, Prospective and Challenges***

Biographical Sketch: *Carlo Segre is the Duchossois Leadership Professor of Physics and Director of the Center for Synchrotron Radiation Research and Instrumentation (CSRRI) at Illinois Institute of Technology (IIT). His research centers around the structure and electronic properties of complex materials including superconducting, magnetic, catalytic, and energy storage materials. Current topics of interest include: structural and electrochemical properties of advanced battery materials; in-situ synchrotron radiation structural studies of catalytic materials for use in fuel cells; structural and electronic properties of magnetoelectric materials and other perovskite materials prepared in the form of nanoparticles and thin films; local structural studies of structural materials for use in nuclear reactors, including in-situ corrosion studies and characterization of nano-crystalline inclusions in steels; development of x-ray optics for synchrotron radiation experimentation.*

As Director of the CSRRI and Deputy Director of both the Materials Research and the Biophysical Collaborative Access Teams which operate experimental facilities at the Advanced Photon Source he is engaged in broadening the use of synchrotron radiation techniques by scientists and engineers. Segre received his bachelor's degrees in Physics and Chemistry from the University of Illinois, Urbana-Champaign in 1976 and his PhD in Physics from University of California, San Diego in 1981. Since 1983 he has been on the faculty at IIT. He is a Fellow of the American Association for the Advancement of Science and of the International Centre for Diffraction Data and has over 120 archival publications.

Thursday Afternoon Plenary Session I: 12:45 PM Thursday, March 3, 2016

Shakeel Kadri, *Executive Director, Center for Chemical Process Safety*

Presentation Title: ***CCPS Vision 20/20 --- A Call To Action***

Biographical Sketch: *Shakeel Kadri was named the Executive Director of the AIChE Center for Chemical Process Safety (CCPS) in 2015. Previous to this role, Shakeel spent 36 years at Air Products and Chemicals, Inc. Most recently he was Director of Global Process Safety and Risk Management, where he was instrumental in building a global process safety team and played a key role in raising the company's process safety risk awareness. Previous to this role, Shakeel served Air Products as global manager, process safety; manager and global leader, process safety; and global quality manager for engineering, manager of process engineering, among other safety, operations and engineering assignments of increasing responsibility.*

Shakeel is a Fellow of both CCPS and AIChE and has served on process safety committees of the American Chemistry Council, the American Petroleum Institute, the Mary Kay O'Connor Process

Safety Center, the International Council of Chemicals Associations, the Compressed Gas Association, the European Industrial Gases and Association, and the American Fuel and Petrochemical Manufacturers Association. He has authored a wide variety of publications, conference papers and a patent. Shakeel earned his bachelor's degree in chemical engineering at the Dharmsinh Desai Institute of Technology of Gujarat University in India, his master's degree in chemical engineering at the Illinois Institute of Technology, Chicago, and an MBA at La Salle University, Philadelphia.

Thursday Afternoon Plenary Session II: 12:45 PM Thursday, March 3, 2016

Linda Broadbelt, *Professor and Chair, Northwestern University*

Presentation Title: ***Mechanistic Modeling of the (Bio)Conversion of (Bio)Macromolecules***

Biographical Sketch: *Linda Broadbelt is Sarah Rebecca Roland Professor in and Chair of the Department of Chemical and Biological Engineering University at Northwestern University. Her research and teaching interests are in the areas of multiscale modeling, complex kinetics modeling, environmental catalysis, novel biochemical pathways, and polymerization/depolymerization kinetics. She is currently the Vice Chair of the Catalysis and Reaction Engineering Division of AIChE, and also previously served on the Executive Board of the National Program Committee of AIChE. She was also appointed to the Scientific Organizing Committee for the 21st and 19th International Symposium on Chemical Reaction Engineering and served on the Science Advisory Committee of the Gulf Coast Hazardous Substance Research Center. She is currently an Associate Editor for Industrial & Engineering Chemistry Research.*

Her honors include selection as the AIChE Women's Initiative Committee Mentorship Excellence Award winner, a Fellow of the American Association for the Advancement of Science, a Fulbright Distinguished Scholar Award, a CAREER Award from the National Science Foundation, a McCormick Excellence Award, appointment to the Defense Science Study Group of the Institute for Defense Analyses, and selection as the Ernest W. Thiele Lecturer at the University of Notre Dame and the Allan P. Colburn Lecturer at the University of Delaware. Linda received her B.S. in chemical engineering from The Ohio State University and graduated summa cum laude. She completed her Ph.D. in chemical engineering at the University of Delaware in 1994 where she was a Du Pont Teaching Fellow in Engineering, a National Science Foundation Graduate Fellow, and a DuPont PhD in Engineering Fellow.

Thursday Dinner Keynote: 7:30 PM Thursday, March 3, 2016

Jeffery Hubbell*, Institute for Molecular Engineering, University of Chicago*

Presentation Title: ***Materials and Protein Engineering for Modulating the Immune System***

Biographical Sketch: *Jeffery Hubbell is the Barry L. MacLean Professor of Molecular Engineering Innovation and Enterprise in the Institute for Molecular Engineering at the University of Chicago. His research focuses on the design of biomaterials to assemble in such a way that they can stimulate the immune systems to fight infection or malignancy, or turn off some aspects of the immune system to address auto-immune diseases such as type-1 diabetes. Hubbell has coined the term "immuno-modulatory materials" to describe this newly emerging field of research.*

Based on his research, Hubbell has founded three companies: Kuros Biosurgery, Anokion, and Focal, Inc.

Hubbell received his bachelor's degree from Kansas State University in 1982, and his PhD from Rice University in 1986, both in chemical engineering. His academic career began at University of Texas and California Institute of Technology. As a professor of biomedical engineering at the Swiss Federal Institute of Technology (ETH) he served as director of the Institute for Biomedical Engineering. Prior to his move to the University of Chicago, Hubbell served as founding director of the Institute of Bioengineering at the École Polytechnique Fédérale de Lusanne (EPFL).

In addition to membership in the National Academy of Engineering, Hubbell is the former president of the Society for Biomaterials. Hubbell is an elected fellow of Biomaterials Science and Engineering, of the American Association for the Advancement of Science, and of the American Institute of Medical and Biological Engineering. Earlier in his career, Hubbell received the W.J. Kolff Award for Outstanding Research from the American Society of Artificial Internal Organs, the Outstanding Dow Young Faculty Award from the American Society of Engineering Education, and the National Science Foundation's Presidential Young Investigator Award.

Friday Morning Keynote: 8:15 AM Friday, March 4, 2016

Corey Correnti, *Senior Vice-President, BP (retired, 2015)*

Presentation Title: ***Energy Infrastructure, Distribution & Trading: Ensuring That Supply Finds Demand***

Biographical Sketch: *Prior to retiring in 2015, Corey held several senior leadership roles at BP. Most recently, Corey was Senior Vice President of Marketing, Sales and Supply where he led the refining crude supply as well as the product supply, sales, and marketing for BP's East of Rockies region. Corey started his career in refining engineering with Amoco in 1985 and later worked in various refining operations management roles. He subsequently led the long term refining planning group which was focused on clean fuels strategies and long term capital support. Corey also worked in BP Chemicals as Global Business Manager for Aromatics, COO for BP's U.S. Product Supply and Trading Operations and Chief of Staff for BP's CFO Office. Corey was President of BP's Supply and Marketing business for the U.S. East and Gulf Coasts and later was head of Supply and Strategy for the East of Rockies Fuels Value Chain. His career has included postings in both the U.K. and U.S. Corey has served as Chair of the American Petroleum Institute's Marketing Subcommittee and BP's Executive Sponsor to the University of Illinois. Corey holds a BS degree in Chemical Engineering from the University of Illinois and an MBA from the University of Chicago. He lives in the Chicago area with his wife Debbie and has one son.*

Friday Afternoon Plenary Session I: 12:45 PM Friday, March 4, 2016

Christopher Burcham*, Senior Engineering Research Advisor, Eli Lilly and Company*

Presentation Title: ***Continuous Processing in the Pharmaceutical Industry: Challenges and Opportunities***

Biographical Sketch: Dr. Christopher Burcham is a Senior Engineering Research Advisor at Eli Lilly and Company, and leads the Particle Design Laboratory in the Small Molecule Design and Development department within Product Research and Development. This group is responsible for the design and development of batch and continuous crystallization processes for all small molecule drug substances currently in development. He is also responsible for spray drying process development for the production of solid dispersions.

Chris received a PhD from Princeton University in 1998, and a BS from the University of Illinois in 1992, both in Chemical Engineering. His career started in Corporate R&D at The Dow Chemical Company transferring later to the Formulation Development group at Dow AgroSciences. In 2002, Chris joined Eli Lilly. Prior to leading the Particle Design Lab, he led the development of chemical processes for a number of late stage molecules.

Chris currently serves on a number of academic Industrial Advisory Boards. He is very active in AIChE, serving regularly as session chair at the annual meeting since 2004, and now Area Chair for Section 2B, Crystallization and Evaporation. He is also a member of the planning committee for the Association of Crystallization Technology.

Friday Afternoon Plenary Session II: 12:45 PM Friday, March 4, 2016

Lorenz T. Biegler, *Professor and Head, Carnegie Mellon University*

Presentation Title: ***Multi-scale Optimization for Chemical Processes***

Biographical Sketch: *Lorenz T. (Larry) Biegler is currently the Bayer University Professor and Head of Chemical Engineering at Carnegie Mellon University. His research interests lie in computer aided process engineering (CAPE) and include flowsheet optimization, optimization of systems of differential and algebraic equations, reactor network synthesis and algorithms for constrained nonlinear process control. He obtained MS and PhD degrees from the University of Wisconsin and his BS degree from the Illinois Institute of Technology, all in chemical engineering.*

Prof. Biegler has been an institute fellow at the National Energy Technology Lab, a visiting scholar at Northwestern University and Lehigh University, a scientist-in-residence at Argonne and Sandia National Labs, a Distinguished Faculty Visitor at the University of Alberta, a Chang Jiang scholar at Zhejiang University, a Gambrinus Fellow at the University of Dortmund, a Fulbright Fellow at the University of Heidelberg, a Distinguished Jubilee Lecturer at IIT-Bombay and the Hougen Visiting Professor at the University of Wisconsin. He is an author on over 300 archival publications and two books. He has edited 11 volumes and given numerous invited presentations at national and international conferences.

He is the recipient of numerous awards including the Lewis Award, McAfee Award (Pittsburgh Section) and the Computers in Chemical Engineering Award, all given by AIChE, Curtis McGraw Research Award and CACHE Computing Award, given by ASEE, the INFORMS Computing Prize, the

Presidential Young Investigator Award from the National Science Foundation, and an honorary doctorate in engineering sciences (Dr.-Ing. e.h.) from the Technical University of Berlin. He is a Fellow of AIChE and SIAM, and a member of ACS, the Mathematical Optimization Society and the National Academy of Engineering.

Friday Afternoon Plenary Session III: 2 PM Friday, March 4, 2016

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

Presentation Title: ***Reactor Internals for Hydro-processing Units***

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.*

Closing Keynote: 6:00 PM Friday, March 4, 2016

Manu Vora, *President, Business Excellence, Inc.*

Presentation Title: ***Sustainable Change Management***

Biographical Sketch: *Dr. Manu Vora is Chairman and President of Business Excellence, Inc., a global quality management consulting firm. He has over 40 years of leadership experience in guiding Fortune 500 companies with Baldrige Performance Excellence assessment in the areas of leadership development, customer satisfaction, employee engagement, and process excellence. Since 1993, he has taught Operations Management courses at various business schools globally. He is connected with over 70 educational institutes world-wide.*

He is a Past Vice President of ASQ, ASQ Fellow, and Certified Quality Engineer. Manu has B.S. (IIT BHU, India, 1968), M.S. and Ph.D. in Chemical Engineering (IIT Chicago - 1970 & 1975), and MBA with Marketing Management (1985). He is a sought after speaker on business excellence and quality management topics with over 525 presentations (including 2013 TEDxIIT Chicago Talk) globally. He has published over 55 articles in professional journals. He has taught Change Management program to government officers in Egypt and shared this presentation world-wide.

Dr. Vora is a Senior Examiner for the Asia Pacific Global Performance Excellence Award Program since 2004. He is recognized with numerous awards from ASQ including Distinguished Service Medal, Grant Medal, Hutchens Medal, Ishikawa Medal, and Lancaster Medal. He is recipient of "2015 Banaras Hindu University Distinguished Alumnus Award". For his social service he has received "2012 IIT Chicago Alumni Medal", "2011 Ellis Island Medal of Honor", and "2010 US President's Volunteer Service Award".

AIChE Midwest Regional Conference

Session Presentations

Thursday, March 3, 2016

Thursday Morning Keynote Session
Thursday, March 3, 2016 (Ballroom)
8:15 AM **LS Chair's Welcome**
Adam Kanyuh (UOP/Honeywell)
8:25 AM **Keynote Introduction**
Hamid Arastoopour (Illinois Institute of Technology)
8:30 AM **High Energy Density Nanoelectrofuel Flow Batteries for Transportation and Renewables: Development, Prospective and Challenges**
Carlo Segre (Illinois Institute of Technology)

Biofuels I
Thursday, March 3, 2016 (Ballroom, **ThA1**)
Chair: *Ignasi Palou-Rivera* (LanzaTech)
Co-Chair: *Jill Jensen* (UOP/Honeywell)
9:45 AM **Low Temperature Hydrogenation of Pyrolytic Lignin over Ru/TiO2: 2D HSQC and 13C NMR Study of Reactants and Products** (ThA1a)
Daniel J. McClelland, Wen Chen, Ali Azarpira, John Ralph, George W. Huber (University of Wisconsin Madison), *Zhongyang Luo* (Zhejiang University)
10:05 AM **Pilot Scale Demonstration of Green Gasoline Production from Woody Biomass** (ThA1b)
Naomi Klinghoffer, Rick Knight, Terry Marker, Jim Wangerow, Pedro Oritz-Toral, Martin Linck, Dan Swanson (Gas Technology Institute)
10:25 AM **Selective Hydrogenolysis of Glycerol into 1,3-propanediol via Highly Crystalline and Mesoporous WO3-Supported Ultrafine Pt Nanocrystals** (ThA1c)
Kai-Chieh Tsao, Yung-Tin Pan, Hong Yang, (University of Illinois at Urbana-Champaign), *Baoliang Lv* (Chinese Academy of Sciences),
10:45 AM **The Influence of Catalysts on Biofuel LCA** (ThA1d)
Pahola Thathiana Benavides, Donald C. Cronauer, Jennifer B. Dunn (Argonne National Laboratory)
11:05 AM **Extract Nitrogen-Containing Compounds in Biocrude Oil Converted from Wet Biowaste via Hydrothermal Liquefaction** (ThA1e)
Karalyn Scheppe, Zhenwei Wu, Wan-Ting Chen, Yuanhui Zhang, Ken Nair (University of Illinois at Urbana-Cahmpaign), *Wanyi Qian* (Stanford University)

Cancer Therapies
Thursday, March 3, 2016 (Armour Dining, **ThA2**)
Chair: *Tim Whitehead* (Michigan State University)
Co-Chair: *Nicholas E. Clay* (University of Illinois at Urbana-Champaign)
9:45 AM **PEGylating Fibronectin Inhibits Tumor Growth and Invasion in an In-Vitro Model** (ThA2a)
Xue Geng, Jialing Xiang, Nancy Karuri (Illinois Institute of Technology)
10:05 AM **High-Throughput Conformational Epitope Mapping to Guide Design of Structure-Based Vaccines** (ThA2b)
Tim Whitehead (Michigan State University)
10:25 AM **Functionalized Flexible Palladium Nanosheets as Patches for HepG2 Cancer Cells** (ThA2c)
Yung-Tin Pan, Cartney E. Smith, Kam Sang Kwok, Jinrong Chen, Hyunjoon Kong, Hong Yang (University of Illinois at Urbana-Champaign)
10:45 AM **Controlled Release of Drug Using Image Contrast Enhancing Nanoparticles** (ThA2d)
Courtney Collins, Madison Taylor, Sara Haworth, ZhanQuan Shi, Zishu Cao, Yoonjee Park (University of Cincinnati)
11:05 AM **Matrix Stiffness and Interstitial Flow Regulate Breast Cancer Malignancy in a Tumor-Microenvironment-on-a-Chip (TMOC) System** (ThA2e)
Nicholas E. Clay, Min Kyung Lee, Hyunjoon Kong (University of Illinois at Urbana-Champaign), *Kyeonggon Shin, Bumsoo Han* (Purdue University)

Process Safety I
Thursday, March 3, 2016 (Alumni Lounge, **ThA3**)
Chair: *Peter Herena* (Baker Engineering and Risk Consultants, Inc.)
Co-Chair: Amy E. Theis (Fauske & Associates)
9:45 AM **PSM Auditing & Lessons Learned to Enhance Overall Business Performance** (ThA3a)
Robert J. Weber (PSRG)
10:05 AM **Inherent Hazards related to Gas Turbine and Steam Turbine Systems in Chemical Processes** (ThA3b)
Stephen Garner, Brenton Cox, Mark Fecke (Exponent)
10:25 AM **Impact of Culture Change on Mechanical Integrity for SIS** (ThA3c)
Murtaza Gandhi (Baker Risk Engineering and Risk Consultants, Inc.)
10:45 AM **Advancing Process Safety** (ThA3d)
Scott M. Wozniak (UOP/Honeywell)
11:05 AM **Latest Developments in Facility Siting (API RP752/753)** (ThA3e)

Ryan Terry, Brian Fagala (PSRG)

Electro-Chemical Processes I
Thursday, March 3, 2016 (Herman Lounge, **ThA4**)
Chair: *Heather Barkholtz* (Northern Illinois University)
Co-Chair: *Jonathan Kucharyson* (University of Michigan)

9:45 AM **An Ambient Temperature Molten Sodium-Vanadium Battery with Aqueous Flowing Catholyte** (ThA4a)
Caihong Liu, Leon Shaw (Illinois Institute of Technology)

10:05 AM **High Performance OER Catalyst of AxByOz Oxidesn** (ThA4b)
Jaemin Kim, Pei-Chieh Shih, Kai-Chieh Tsao, Xi Yin, Hong Yang (University of Illinois at Urbana-Champaign)

10:25 AM **The Origin of Electrochemical Activity of Cobalt Oxide Water Oxidation Catalytic Amorphous Thin Film** (ThA4c)
Gihan Kwon, Anil Mane, Alex B. Martinson, David M. Tiede (Argonne National Laboratory), *Hacksung Kim, Jonathan D. Emery* (Northwestern University)

10:45 AM **Investigation of Oxygen Generation During Li-ion Battery Operation Using In-situ Fluorescence Spectroscopy** (ThA4d)
Mo Li, Javier Parrondo, Vijay Ramani (Illinois Institute of Technology)

11:05 AM **Selective Electrochemical Detection of Ciprofloxacin with a Porous Nafion/Multi-Walled Carbon Nanotube Composite Film Electrode** (ThA4e)
Pralay Gayen, Brian P. Chaplin (University of Illinois at Chicago)

Process Design and Optimization I
Thursday, March 3, 2016 (Crown Room, **ThA5**)
Chair: *Juan Salazar* (UOP/Honeywell)
Co-Chair: *Mustafa Cagdas Ozturk* (Illinois Institute of Technology)

9:45 AM **A Multi-Objective Optimization Approach to Optimal Sensor Location Problem in IGCC Power Plants** (ThA5a)
Pallabi Sen, Kinnar Sen (University of Illinois at Chicago), Dr. Urmila Diwekar (Vishwamitra Research Institute)

10:05 AM **Profit Based Sensor Network Design Revisited: Application of the Generalized Bender Decomposition** (ThA5b)
Jin Zhang, Donald J. Chmielewski (Illinois Institute of Technology)

10:25 AM **A Nonlinear Optimization Approach to the Estimation of Spatial Transmission Parameters in Infectious Disease Spread** (ThA5c)
Todd Zhen, Carl D. Laird (Purdue University)

10:45 AM **An Efficient Superstructure Generation and Modeling Framework** (ThA5d)
WenZhao (Tony) Wu, Carlos A. Henao, Christos T. Maravelias (University of Wisconsin Madison)

11:05 AM **Novel Sampling Technique for High Dimensional Stochastic Optimization Problem** (ThA5e)
Nishant Dige, Urmila Diwekar (University of Illinois at Chicago)

Thursday Plenary Session I
Thursday, March 3, 2016 (Ballroom)

12:45 PM **Plenary Introduction**
Harold Kung (Northwestern University)

12:55 PM **Mechanistic Modeling of the (Bio)Conversion of (Bio)Macromolecules**
Linda Broadbelt (Northwestern University)

Thursday Plenary Session II
Thursday, March 3, 2016 (Armour Dining)

12:45 PM **Plenary Introduction**
Brenton L. Cox (Exponent Inc.)

12:55 PM **CCPS Vision 20/20 --- A Call To Action**
Shakeel Kadri (AIChE Center for Chemical Process Safety)

Biofuels II
Thursday, March 3, 2016 (Ballroom, **ThB1**)
Chair: *Eric Doskocil* (BP)
Co-chair: *Dan McClelland* (University of Wisconsin)

2:00 PM **Biocomposites for Algae Production** (ThB1a)
Omar Khalil, Reza Ghodsi, Bader Jarai, Fouad Teymour (Illinois Institute of Technology)

2:20 PM **Techno-Economic and Environmental Life Cycle Assessments of Hydrocarbon Biofuel from Poplar** (ThB1b)
David Shonnard, Olumide Winjobi, Wen Zhou, Paul Langford, Ezra Bar Ziv (Michigan Technological University)

2:40 PM **Greenhouse Gas Emissions of Ethanol Production Via the LanzaTech Process from Biomass Cellulosic and Waste Gas Feedstocks** (ThB1c)
Ignasi Palou-Rivera (LanzaTech), *Robert Handler* (Michigan Technological University)

3:00 PM **Production of Transportation Fuels by Co-Processing Biomass-Derived Pyrolysis Oils in a Petroleum Refinery Fluid Catalytic Cracking Unit** (ThB1d)
Jill R. Jensen, Chad R. Huovie, Stanley J. Frey (UOP/Honeywell)

3:20 PM **Upgradation of Biocrude Oil Converted from Bio-Wastes via Hydrothermal Liquefaction into Drop-in Fuel and Value-Added Chemicals** (ThB1e)
Wan-Ting Chen, Yuanhui Zhang, Peng Zhang (University of Illinois at Urbana-Champaign), *Lance Schideman, B.K. Sharma* (Illinois Sustainability Technology Center)

Drug Delivery I
Thursday, March 3, 2016 (Armour Dining, **ThB2**)
Chair: *Haipeng Lui* (Wayne State University)
Co-chair: *Benjamin M King* (University of Iowa)

2:00 PM **Exploring the Possibility of Exploiting Protein Corona for Targeted Nanoparticle Delivery** (ThB2a)
Vahid Mirshafiee, Raehyun Kim, Soyun Park, Mary L. Kraft (University of Illinois at Urbana-Champaign), *Morteza Mahmoudi* (Stanford University)

2:20 PM **Effect of PEGylated Gold Nanoparticle Permeation on lipid bilayer membranes** (ThB2b)
Priyanka A. Oroskar, Cynthia Jameson (University of Illinois at Chicago), Sohail Murad (Illinois Institute of Technology)

2:40 PM **Development of a Photoresponsive Scaffold Composed of Self-Assembled Nanostructures** (ThB2c)
Nicholas Karabin, Evan Scott (Northwestern University)

3:00 PM **Polyphosphate loaded Nanoparticles for Suppression of Bacterial Collagenase and Intestinal Healing** (ThB2d)
Dylan Nichols, Fouad Teymour, Georgia Papavasiliou (Illinois Institute of Technology), *Melissa Arron, Olga Zaborina, John Alverdy* (University of Chicago)

3:20 PM **Photo-Click Hydrogels Prepared from Functionalized Cyclodextrin and Poly(ethylene glycol) for Drug Delivery and In-Situ Cell Encapsulation** (ThB2e)
Han Shih, Chien-Chi Lin (Purdue University)

Process Safety II
Thursday, March 3, 2016 (Alumni Lounge, **ThB3**)
Chair: *Scott Wozniak* (UOP/Honeywell)
Co-chair: *Jesse Calderon* (Baker Engineering and Risk Consultants, Inc.)

2:00 PM **Five Steps to Managing Combustible Dust Hazards** (ThB3a)
Amy Theis (Fauske & Associates, LLC)

2:20 PM **CFD Based Thermal Fatigue Risk Assessment in Refinery Process Lines** (ThB3b)
Raj Venuturumilli, Madhusuden Agrawal, Samir Khanna (BP)

2:40 PM **Extending the Life of a High Temperature Refinery Reactor** (ThB3c)
Jerry Wilks (CITGO Petroleum Inc.)

3:00 PM **A Maturity Model for Assessing your Company's PSM Program** (ThB3d)
Madonna Breen (PSRG)

3:20 PM **LOPA and the Art of Motorcycle Maintenance** (ThB3e)
Peter Herena (Baker Risk Engineering and Risk Consultants)

Electro-Chemical Processes II
Thursday, March 3, 2016 (Herman Lounge, **ThB4**)
Chair: *Gihan Kwon* (Argonne National Laboratory)
Co-chair: *Canan Acar* (University of Ontario Institute of Technology)

2:00 PM **Electrodeposition of Copper for Metamaterial Fabrication** (ThB4a)
Shendu Yang (University of Missouri)

2:20 PM **Engineering Nanofluid Electrodes: Control of Rheology and Electrochemical Activity of Nickel Hydroxide Nanoparticles** (ThB4b)
Elahe Moazzen, Carlo Segre (Illinois Institute of Technology), *Sujat Sen, Chun Man Chow, Elena Timofeeva* (Argonne National Lab)

2:40 PM **Characterization of Electronic and Structural Transitions for V(acac)3- and Ru(acac)3-based Flow Battery Electrolytes Using X-Ray Absorption Spectroscopy** (ThB4c)
Jonathan Kucharyson, Jason Gaudet, Brian Wyvratt, Levi Thompson (University of Michigan)

3:00 PM **Rational Design of Low Cost Electrode Catalysts for Fuel Cell Applications** (ThB4d)
Heather M. Barkholtz (Northern Illinois University), *Lina Chong, Zachary B. Kaiser, Di-Jia Liu* (Argonne National Laboratory)

3:20 PM **Environmental Transmission Electron Microscopy Study of Composition Redistribution for Pt-Ni Octahedral Electrocatalysts for Reduction of Oxygen** (ThB4e)
Yung-Tin Pan, Jianbo Wu, Hong Yang (University of Illinois at Urbana-Champaign)

Multiphase CFD Tutorial
Thursday, March 3, 2016 (Crown Room, **ThB5**)
Chair: *Reza Mostofi* (UOP/Honeywell)

2:00 PM **Multiphase Conservation Laws and Their Constitutive Equations** (ThB5a)
Dimitri Gidaspow (Illinois Institute of Technology)

3:45 PM **Demonstration of IIT Multiphase CFD Code for Reactor Improvement** (ThB5b)
Dimitri Gidaspow (Illinois Institute of Technology)

The Hydrogen Economy
Thursday, March 3, 2016 (Ballroom, **ThC1**)
Chair: *David Shonnard* (Michigan Technological University)
Co-chair: *Jui-Kun Peng* (Argonne National Laboratory)

4:00 PM **A Fifty+ Year Perspective on Sustainability** (ThC1a)
Robert Anderson (Illinois Institute of Technology)

4:20 PM **Experimental Investigation of a Hybrid Photoelectrochemical Hydrogen Production System** (ThC1b)
Canan Acar, Ibrahim Dincer (University of Ontario Institute of Technology)

4:40 PM **NaBH4 “Wrapped in Graphene”: Significantly Improved the Hydrogen Storage Capacity and Reversibility through Nanoencapsulation** (ThC1c)

Lina Chong (Argonne National Laboratory)

5:00 PM **Mechanical Property Study of Metal-Organic Framework** (ThC1d)
Zhi Su, Kenneth Suslick (University of Illinois at Urbana-Champaign)

5:20 PM **Low-Temperature Preferential Oxidation of Carbon Monoxide on Pt3Ni Alloy Nanoparticle Catalyst with Engineered Surface** (ThC1e)
Zhenmeng Peng, Sang Youp Hwang, Eric Yurchekfrodl, Changlin Zhang (University of Akron)

Drug Delivery II

Thursday, March 3, 2016 (Armour Dining, **ThC2**)
Chair: *Georgia Papavasiliou* (Illinois Institute of Technology)
Co-chair: *Brittany Hartwell* (University of Kansas)

4:00 PM **Agrochemical likeliness: Why Agrochemicals Differ from Drugs?** (ThC2a)
Saurabh Shukla (University of Illinois at Urbana-Champaign)

4:20 PM **Antibiotic Probiotics Reduce Salmonella in GI Tract of Animals** (ThC2b)
Yiannis Kaznessis, Brittany Forkus, Kathryn Geldart (University of Minnesota)

4:40 PM **Engineering Albumin-hitchhiking Vaccines for Type 1 Diabetes** (ThC2c)
Haipeng Liu, Meng Li, Jingchao Xi (Wayne State University)

5:00 PM **Drug Selectivity Mechanism of Kinases** (ThC2d)
Zahra Shamsi, Diwakar Shukla (University of Illinois at Urbana-Champaign)

5:20 PM **The Role of Natural Fluids in Studies of In-Vitro Pulmonary Drug Delivery** (ThC2e)
Benjamin King, Jennifer Fiegel (University of Iowa)

Process Safety III

Thursday, March 3, 2016 (Alumni Lounge, **ThC3**)
Chair: *Robert J. Weber* (PSRG)
Co-chair: *Brenton L. Cox* (Exponent Inc.)

4:00 PM **Quantitative Risk Assessment Technological Advancements** (ThC3a)
Jesse Calderon (Baker Risk Engineering and Risk Consultants, Inc.)

4:20 PM **Using Bow Ties for Process Hazards Analysis** (ThC3b)
Ngoc (Annie) Nguyen (PSRG)

4:40 PM **Combining Traditional UOP HAZOP Analysis with Dynamic Simulation a New Process Safety / Risk Assessment Tool** (ThC3c)
Scott M. Wozniak (UOP)

5:00 PM **A Comparison of Water Distribution Resilience Metrics** (ThC3d)
Michael Bynum, Carl Laird (Purdue University), Terra Haxton, Regan Murray (Environmental Protection Agency), Katherine Klise (Sandia National Laboratories)

5:20 PM **Chemical Facility Anti-Terrorism Standards, 6 CFR part 27** (ThC3e)
Gregory Wolff (U.S. Homeland Security)

Process Design and Optimization II

Thursday, March 3, 2016 (Herman Lounge, **ThC4**)
Chair: *Urmila Diwekar* (Vishwamira Research Institute)
Co-chair: *Rajesh Gattupalli* (UOP/Honeywell)

4:00 PM **Design and Characterization of a Millifluidic Herringbone Mixer** (ThC4a)
Joseph Whittenberg, Vivek Kumar, Keegan Lane, Sumit Verma, Heeral, Paul J. A. Kenis (University of Illinois at Urbana-Champaign)

4:20 PM **A Parallel Dynamic Optimization Approach for Inverse Problems in Water Distribution Systems** (ThC4b)
Jose Rodriguez, Carl D. Laird (Purdue University)

4:40 PM **Heterogeneous Multi-Agent Optimization Framework to Solve Large Scale Process System Engineering Problems** (ThC4c)
Berhane H. Gebreslassie, Urmila M. Diwekar (Vishwamitra Research Institute)

5:00 PM **Numerical Optimization of Gasoline Storage Tank Ventilation** (ThC4d)
Chenn Zhou, Bin Wi (Purdue University Calumet)

5:20 PM **A Novel Approach to Improve the Barrier Properties of Polyethylene Terephthalate** (ThC4e)
Kazem Majdzadeh Ardakani, Saleh A. Jabarin (University of Toledo)

Job Search Strategies (*Laptops Recommended*)

Thursday, March 3, 2016 (Armour Conference Room, **ThC5**)
Chair: *BJ Engelhardt* (Illinois Institute of Technology)

4:00 PM **Finding Your Market** (ThC5a)
Akshar Patel (Illinois Institute of Technology)

4:55 PM **Making Your Connections** (ThC5b)
Akshar Patel (Illinois Institute of Technology)

Poster Session

Thursday, March 3, 2016 (Gallery Lounge)
Chair: *Satish Parulekar* (Illinois Institute of Technology)
Co-Chair: *Seok Hoon Hong* (Illinois Institute of Technology)

5:45 PM **Poster Session**

Local Section Dinner and Dinner Keynote

Thursday, March 3, 2016 (Ballroom)

6:30 PM **Dinner**

7:15 PM **Local Section Announcements**
Adam Kanyuh (UOP/Honeywell)

7:25 PM **Keynote Introduction**
Georgia Papavasiliou (Illinois Institute of Technology)

7:30 PM **Materials and Protein Engineering for Modulating the Immune System**
Jeffery Hubbell (University of Chicago)

AIChE Midwest Regional Conference
Session Presentations
Friday, March 4, 2016

Friday Morning Keynote Session
Friday, March 4, 2016 (Ballroom)
8:15 AM **Recognition for Volunteers from the GAC Chair**
Patrick Shannon (Middough Inc.)
8:25 AM **Keynote Introduction**
Paul Kenis (University of Illinois at Urbana-Champaign)
8:30 AM **Energy Infrastructure, Distribution & Trading: Ensuring That Supply Finds Demand**
Corey Correnti (BP, retired 2015)

Process Modeling and Estimation
Friday, March 4, 2016 (Ballroom, **FrA1**)
Chair: *Jeffrey M. Zalc* (BP)
Co-Chair: *Alexander Dowling* (University of Wisconsin)
9:45 AM **A Meal Detection and Carbohydrate Estimation Algorithm Based on CGM Data for Use in AP Systems** (FrA1a)
Sadiqeh Samadi, Kamuran Turksoy, Jianyuan Feng, Iman Hajzadeh, Mert Sevil, Ali Cinar (Illinois Institute of Technology)
10:05 AM **Real-Time Estimation of Plasma Insulin Concentration Using Glucose Measurements in Patients with Type 1 Diabetes (FrA1b)**
Iman Hajizadeh,Kamuran Turksoy, Sadiqeh Samadi, Jianyuan Feng, Mert Sevil, Ali Cinar (Illinois Institute of Technology)
10:25 AM **A Simulation Model Assessing the Integration of a Cold Thermal Energy Storage (TES) into an Air Conditioning System** (FrA1c)
Ahmed Aljehani, Said Al-Hallaj (University of Illinois at Chicago), *Siddique Khateeb* (AllCell Technologies)
10:45 AM **Population Balance Modeling of Mechanical Dispersion of semi-solid binders in High Shear Wet Granulation** (FrA1d)
Sudarshan Ganesh, Nathan J. Davis, James D. Litster (Purdue University)
11:05 AM **Modeling and Optimization of Spherical Crystallization through a Coupled Population Balance Framework** (FrA1e)
Ramon Pena, Zoltan K. Nagy, Doraiswami Ramkrishna (Purdue University), *Christopher L. Burcham, Daniel J. Jarmer* (Eli Lilly & Co.)

Tissue Engineering I
Friday, March 4, 2016 (Armour Dining, **FrA2**)
Chair: *Nancy Karuri* (Illinois Institute of Technology)
Co-Chair: *Ashty Karim* (Northwestern University)
9:45 AM **Effect of Fibronectin on the Diffusion and Rigidity of the Fibrin-Fibronectin Matrix** (FrA2a)
Chengyao Wang, Nancy W. Karuri (Illinois Institute of Technology)
10:05 AM **MR Tools for the Assessment of Cartilage and Osteochondral Tissue Engineering (FrA2b)**
Mrignayani Kotecha (University of Illinois at Chicago)
10:25 AM **Agent-Based Modeling of Scaffold Vascularization and Bone Tissue Regeneration Using Biodegradable Polymer/Ceramic Composite** (FrA2c)
Chenlin Lu, Elif S. Bayrak, Mustafa C. Ozturk, Banu Akar, Eric M. Brey, Ali Cinar (Illinois Institute of Technology)
10:45 AM **Synthesis and Characterization and In-Vivo Efficacy of a Lubricin Mimic to Reduce Progression of Osteoarthritis** (FrA2d)
Jim McMasters, Alyssa Panitch, Shaili Sharma (Purdue University), *Corey P. Neu* (University of Colorado, Boulder), *Alexandra Lawrence* (Biomet)
11:05 AM **Manipulating Focal Adhesion Formation by Nanotopographical Substrates for Enhanced Myogenic Differentiation of Primary Myoblasts** (FrA2e)
Eunkyung Ko, Hyunjoon Kong (University of Illinois at Urbana-Champaign), *Seung-Jung Yu, Sung Gap Im* (Korea Advanced Institute of Science and Technology)

Refining and Petrochemical Engineering I
Friday, March 4, 2016 (Alumni Lounge, **FrA3**)
Chair: *Paolo Palmas* (UOP/Honeywell)
Co-Chair: *Emad Ghadirian* (Illinois Institute of Technology)
9:45 AM **Maximizing Diesel Production in an FCC Refinery** (FrA3a)
Ron Subris (UOP/Honeywell)
10:05 AM **Numerical Simulation of an Industrial Fluid Catalytic Cracking Regenerator** (FrA3b)
Chenn Zhou, Bin Wu, Guangwu Tang, Armin Silaen (Purdue University - Calumet)
10:25 AM **Improving Refinery Unit Start-ups and Shut Downs** (FrA3c)
Jerry Wilks (CITGO Petroleum)
10:45 AM **Dividing-Wall Column Screening Guidelines and Applications** (FrA3d)
Robert Tsai, Paul Steacy, Xin X. (Frank) Zhu (UOP/Honeywell)
11:05 AM **Performance of Petrochemical Buildings Subject to Fire Hazards** (FrA3e)

Ernesto Gasulla (Baker Risk Engineering and Risk Consultants, Inc.)

Environmental Engineering

Friday, March 4, 2016 (Herman Lounge, **FrA4**)
Chair: *Gerardo J. Ruiz-Mercado* (U.S. EPA)
Co-Chair: *Jarad L. Champion* (Geosyntec Consultants)

9:45 AM **Improving Resource Availability for Sustainable Manufacturing: Review and Case Study on Phosphorus** (FrA4a)
Daniel Bampoh, Shweta Singh (Purdue University)

10:05 AM **Electrochemical Impedance Spectroscopy Study of Membrane Fouling and Electrochemical Regeneration at a sub-Stoichiometric TiO2 Reactive Electrochemical Membrane** (FrA4b)
Yin Jing, Lun Guo, Brian P. Chaplin (University of Illinois at Chicago)

10:25 AM **Detecting Heavy Metals in Water using Carbon Nanotube Threads** (FrA4c)
David Siebold, Vesselin Shanov, William R. Heineman, Noe Alvarez, Daoli Zhao (University of Cincinnati)

10:45 AM **Removal of Phenol from Produced Water Utilizing a NiO-based Catalyst in Supercritical Water** (FrA4d)
Chamara De Silva, Jason Trembly (Ohio University)

11:05 AM **Design of Novel Polymeric Adsorbents for Metal Ion Removal from Water Using CAMD** (FrA4e)
Urmila Diwekar, Rajib Mukherjee, Berhane Gebreslassie (Vishwamitra Research Institute)

Fluid Properties and Transport Phenomena

Friday, March 4, 2016 (Crown Room, **FrA5**)
Chair: *Lewis Wedgewood* (University of Illinois at Chicago)
Co-Chair: *Joseph Whittenberg* (University of Illinois at Urbana-Champaign)

9:45 AM **Microfluidic Mixing to Prepare Polyaspartamide Nanoparticles** (FrA5a)
Nicholas E. Clay, Joseph J. Whittenberg, Vivek Kumar, Jinrong Chen, Paul Kenis, Hyunjoon Kong (University of Illinois at Urbana-Champaign)

10:05 AM **The Role of Additives and Orientation on the Gas Transport Properties of Poly (Ethylene Terephthalate)** (FrA5b)
Shahab Zekriardehani, Maria R. Coleman, Saleh A. Jabarin (University of Toledo)

10:25 AM **Application of Non-uniform Magnetic Fields on Ferrofluid Colloidal Dispersions using an Iterative Constraint Method: A Brownian Dynamics Study** (FrA5c)
Sean Dubina, Lewis Wedgewood (University of Illinois at Chicago)

10:45 AM **Effects of Salt on the Stratification and Dynamics of Foam Films** (FrA5d)
Rabees Rafiq, Vivek Sharma, Subinuer Yilixiati (University of Illinois at Chicago)

11:05 AM **Molecular Modeling of Isopropanol Dehydration Using Molecular Simulations in the Presence of Contaminants** (FrA5e)
Xiaoyu Wang, Sohail Murad (Illinois Institute of Technology)

Friday Plenary Session I

Friday, March 4, 2016 (Ballroom)

12:45 PM **Plenary Introduction**
Carl Laird (Purdue University)

12:50 PM **Multi-scale Optimization for Chemical Processes**
Lorenz T. Biegler (Carnegie Mellon University)

Friday Plenary Session II

Friday, March 4, 2016 (Armour Dining)

12:45 PM **Plenary Introduction**
Zoltan Nagy (Purdue University)

12:50 PM **Continuous Processing in the Pharmaceutical Industry: Challenges and Opportunities**
Christopher Burcham (Eli Lilly & Co.)

Friday Plenary Session III

Friday, March 4, 2016 (Alumni Lounge)

1:55 PM **Plenary Introduction**
Marty Duran (BP)

2:00 PM **Reactor Internals for Hydroprocessing Units**
Henrik Rasmussen (Haldor Topsoe, Inc.)

Process Operations and Control

Friday, March 4, 2016 (Ballroom, **FrB1**)
Chair: *Alexander Dowling* (University of Wisconsin)
Co-Chair: *Jin Zhang* (Illinois Institute of Technology)

2:00 PM **Optimal Control of Batch Distillation with Missing Components** (FrB1a)
Urmila Diwekar (Vishwamitra Research Institute)

2:20 PM **Hybrid Online Sensor Error Detection and Functional Redundancy for Systems with Time-Varying Parameters** (FrB1b)
Jianyuan Feng, Kamuran Turksoy, Sediqeh Samadi, Iman Hajizadeh, Mert Sevil, Ali Cinar (Illinois Institute of Technology)

2:40 PM **Design of Dynamic Systems based on Efficient Ant Colony Optimal Control (EACOC) Algorithm: Case Study Chemical Process Control** (FrB1c)
Berhane H. Gebreslassie, Urmila M. Diwekar (Vishwamitra Research Institute)*, Gaurav Mirlekar, Fernando V. Lima* (West Virginia University)

3:00 PM **Mixed-Integer Programming Solution Methods for Inventory Routing Problems** (FrB1d)
Yachao Dong, Chirstos T. Maravelias (University of Wisconsin Madison), *Jose M. Pinto, Arul Sundaramoorthy* (Praxair, Inc.)

3:20 PM **On the Alleviation of Inventory Creep in Process Scheduling** (FrB1e)

Yazeed Aleissa, Donald J. Chmielewski (Illinois Institute of Technology)

Tissue Engineering II

Friday, March 4, 2016 (Armour Dining, **FrB2**)
Chair: *Mrignayani Kotecha* (University of Illinois at Chicago)
Co-Chair: *Chenlin Lu* (Illinois Institute of Technology)

2:00 PM **Macrophage Activation and Reprogramming is Dependent on Crosslinking Density of Hyaluronan Hydrogels** (FrB2a)
Jamie E. Rayahin, Richard A. Gemeinhart (University of Illinois at Chicago)

2:20 PM **Tether Strength of Cell Adhesion Ligands Modulates Biological Activities of a Cell-Laden Hydrogel** (FrB2b)
Jooyeon Park, Min Kyung Lee, Xuefeng Wang, Mehdi Roein-Peikar, Taekjip Ha, Hyujoon Kong (University of Illinois at Urbana-Champaign)

2:40 PM **Development of Hydrogel Nanoparticles for Sustained Delivery of Angiogenic Peptides** (FrB2c)
Daniel A. Young, Marja Bittencourt, Luana Dias, Wesley Lo, Fouad Teymour, Georgia Papavasiliou (Illinois Institute of Technology)

3:00 PM **Multivalent Nanomaterial Arrays Leverage Antigen Specificity to Modulate Immune Response in Autoimmune Disease** (FrB2d)
Brittany Hartwell, Heather Shinogle, Bradley Sullivan, Laura Northrup, Cory Berkland (University of Kansas)

3:20 PM **Modular Crosslinking of Gelatin Based Thiol-Norbornene Hydrogels for In-Vitro 3D Culture of Hepatocellular Carcinoma Cells** (FrB2e)
Tanja Greene, Chien-Chi Lin (Purdue University)

Refining and Petrochemical Engineering II

Friday, March 4, 2016 (Alumni Lounge, **FrB3**)
Chair: *Victor Sussman* (Dow Chemical Company)
Co-Chair: *Juan Salazar* (UOP/Honeywell)

2:00 PM **Reactor Internals for Hydroprocessing Units** (FrB3a)
Henrik Rasmussen (Haldor Topsoe, Inc.)

2:40 PM **Hydroprocessing Revamps for Maximum Flexibility and Profitability** (FrB3c)
Sudhakar Chakka, Laura Kadlec (UOP)

3:00 PM **Maximizing Reliability and Profitability in Hydrogen Plant Designs** (FrB3d)
Diane Dierking (Johnson Matthey Process Technologies)

3:20 PM **Methanol to Olefins (MTO) - Market and Technology Review** (FrB3e)
Joseph Montalbano (UOP)

Pharmaceutical Processing

Friday, March 4, 2016 (Herman Lounge, **FrB4**)
Chair: *Hamid Arastoopour* (Illinois Institute of Technology)
Co-Chair: *Vahid Mirshafiee* (University of Illinois at Urbana-Champaign)

2:00 PM **Optimization of Batch and Continuous Cooling Crystallization of High Aspect Ratio Crystals under Nucleation, Growth, Dissolution and Breakage for Shape Control** (FrB4a)
David Acevedo, Zoltan K. Nagy (Purdue University), *Christopher L. Burcham, Daniel J. Jarmer* (Eli Lilly & Co.)

2:20 PM **Analyzing the Effect of Material Properties on a Twin Screw Wet Granulation Process** (FrB4b)
Shankali Pradhan, Maitraye Sen, Carl Wassgren, James Litster (Purdue University), *Ian Gabbott, Gavin Reynolds* (AstraZeneca)

2:40 PM **Estimation of the Breakage and Selection Function in the Roller Compaction Process** (FrB4c)
Mariana Moreno, Sudarshan Ganesh, Gintaras V. Reklatis, Zoltan K. Nagy, Alexander R. Milaszewski, Isaac E. Mendoza (Purdue University)

3:00 PM **Development of Drug Nanocrystals for Intravenous Injection** (FrB4d)
Tonglei Li (Purdue University)

3:20 PM **Application of Automated Direct Nucleation Control in Continuous Cooling Crystallization and Wet Milling Processes** (FrB4e)
Yang Yang, Liangcheng Song, Zoltan K. Nagy (Purdue University)

(Canceled) Process Safety Workshop I

~~Friday, March 4, 2016 (Crown Room, **FrB5**)~~
Chair: *Brenton L. Cox* (Exponent Inc.)
Co-Chair: *Peter Hereña* (Baker Engineering and Risk Consultants, Inc.)

(Canceled) 2:00 PM **Process Hazards Analysis** (FrB5a)
Peter Hereña (Baker Engineering and Risk Consultants, Inc.)

(Canceled) 2:55 PM **Safe Work Practices** (FrB5b)
Brenton Cox, Sean Dee (Exponent Inc.)

Leadership Workshop

Friday, March 4, 2016 (Armour Conference Room, **FrB6**)
Chair: *Alfred Nunez* (Illinois Institute of Technology)

2:00 PM **Interactive Workshop on Leadership Excellence** (FrB6a)
Manu Vora (Business Excellence Inc.)

Sustainable Power Systems

Friday, March 4, 2016 (Ballroom, **FrC1**)
Chair: *Dennis O'Brien* (Jacobs Consultancy)
Co-Chair: *Yazeed Aleissa* (Illinois Institute of Technology)

4:00 PM **Numerical Modeling of CO_2 Desorption Process in a Carbon Capture Unit using the Fluidized Bed Process** (FrC1a)
Emad Ghadirian, Hamid Arastoopour, Javad Abbasian (Illinois Institute of Technology)

4:20 PM **High-Gravity Carbonation Process for Carbon Capture and Utilization Exemplified by Steelmaking Industry** (FrC1b)
Shu-Yuan Pan, Silu Pei, Pen-Chi Chiang (National Taiwan University), *Yupo J. Lin* (Argonne National Laboratory), *Yi-Hung Chen* (National Taipei University of Technology)

4:40 PM **Exploiting Electricity Markets for Better Systems Engineering** (FrC1c)
Alexander Dowling, Victor Zavala (University of Wisconsin Madison)

5:00 PM **On the Use of Multistage Stochastic Programming for the Design of Grid Scale Energy Storage Systems** (FrC1d)
Oluwasanmi Adeodu, Donald J. Chmielewski (Illinois Institute of Technology)

5:20 PM **Optimal Design and Control of CCHP Systems for Housing Complexes** (FrC1e)
Luis Fabián Fuentes Cortés, José Maria Ponce Ortega (Universidad Michoacana de San Nicolás de Hidalgo), *Alexander Dowling, Victor M. Zavala Tejeda* (University of Wisconsin Madison)

__Modeling of Biological Systems__
Friday, March 4, 2016 (Armour Dining, **FrC2**)
Chair: *Seok Hoon Hong* (Illinois Institute of Technology)
Co-Chair: *Daniel Young* (Illinois Institute of Technology)

4:00 PM **Spatio-Temporal Engineering of Biochemical Reaction Networks** (FrC2a)
Milan Mrksich (Northwestern University)

4:20 PM **High Definition (HD) Fourier Transform Infrared (FT-IR) Spectroscopic Imaging for Rapid Chemical Analysis** (FrC2b)
Shachi Mittal, Rohit Bhargava (University of Illinois at Urbana-Champaign)

4:40 PM **Modeling and Prediction of Antibody Production in Mammalian Cell Culture - Dual Rate Approach** (FrC2c)
Jingwei Gan, Satish J. Parulekar, Ali Cinar (Illinois Institute of Technology)

5:00 PM **A Cell-Free Framework for Rapid Biosynthetic Pathway Prototyping and Enzyme Discovery** (FrC2d)
Ashty Karim, Michael Jewett (Northwestern University)

5:20 PM **Development of a Dynamic Cell-Free Model of B. Subtilis Metabolism** (FrC2e)
Michael Vikhovoy, Jeffrey Varner (Purdue University)

__CFD Methods and Applications__
Friday, March 4, 2016 (Alumni Lounge, **FrC3**)
Chair: *Hadjira Iddir* (UOP/Honeywell)
Co-Chair: *Raj Venuturumilli* (BP)

4:00 PM **Computational Fluid Dynamics (CFD) for Equipment Design and Development** (FrC3a)
Quan Yuan, Reza Mostofi-Ashtiani, Hadjira Iddir (UOP/Honeywell)

4:20 PM **Four Phase Flow Model for Methane Production from an Unconsolidated Gas Hydrate Reservoir** (FrC3b)
Deniz Hinz, Hamid Arastoopour (Illinois Institute of Technology)

4:40 PM **Computational Fluid Dynamics for FCC: Opportunities and Challenges** (FrC3c)
Raj Venuturumilli (BP)

5:00 PM **Liquid Maldistribution Study of Rocking FLNG Columns using Computational Fluid Dynamics** (FrC3d)
Pengfei Chen (UOP/Honeywell)

5:20 PM **CFD Fluidized Bed Reactor Design 1. For Diesel from Shale Gas 2. For Silicon for Solar Cells** (FrC3e)
Dimitri Gidaspow (Illinois Institute of Technology)

__Environmentally Conscious Process Design__
Friday, March 4, 2016 (Herman Lounge, **FrC4**)
Chair: *Pahola Thathiana Benavides* (Argonne National Laboratory)
Co-Chair: *Daniel Bampoh* (Purdue University)

4:00 PM **Lessons Learned When Evaluating the Feasibility of Emerging Green Technologies** (FrC4a)
Sean J. Dee, Russell A. Ogle (Exponent)

4:20 PM **Thermal Energy Storage Device for Space Cooling Applications** (FrC4b)
Siddique Khateeb, Mukund Bhaskar, Said Al-Hallaj (AllCell Tehcnologies)

4:40 PM **Developing and Analyzing Chemical Process Data for Life Cycle Inventories and Sustainability Evaluation** (FrC4c)
Gerado J. Ruiz-Mercado, Raymond L. Smith, Michael A. Gonzalez (US EPA)

5:00 PM **Valuing Water in Rankine Cycle Power Generation** (FrC4d)
Suresh Jambunathan (Veolia)

5:20 PM **Prospective Life-cycle Technology Assessment Modeling Framework for Sustainable Chemical Production** (FrC4e)
Yuan Yao, Eric Masanet (Northwestern University), *Diane Graziano, Matthe Riddle* (Argonne National Laboratory), *Joe Cresko* (US DOE)

(Canceled) __Process Safety Workshop II__
~~Friday, March 4, 2016 (Crown Room, **FrC5**)~~
Chair: *Peter Hereña* (Baker Engineering and Risk Consultants, Inc.)
Co-Chair: *Brenton L. Cox* (Exponent Inc.)

(Canceled) 4:00 PM **Quantitative Risk Analysis** (FrC5a)
Jesse Calderon, Mike Toraason (Baker Engineering and Risk Consultants, Inc.)

(Canceled) 4:55 PM **Standard Operating Procedures** (FrC5b)
Sunil Lakhiani, Sean Dee (Exponent Inc.)

__Closing Keynote and Reception__
Friday, March 4, 2016 (Ballroom)

5:45 PM **Invitation to MRC 2017**
Donald J. Chmielewski (Illinois Institute of Technology)

5:55 PM **Keynote Introduction**
Sohail Murad (Illinois Institute of Technology)

6:00 PM **Sustainable Change Management**
Manu Vora (Business Excellence Inc.)

AIChE Midwest Regional Conference
Keynote and Plenary Abstracts

Thursday Morning Keynote Session

Thursday, March 4, 2016 (Ballroom)

8:15 AM **LS Chair's Welcome**
Adam Kanyuh (UOP/Honeywell)

8:25 AM **Keynote Introduction**
Hamid Arastoopour (Illinois Institute of Technology)

8:30 AM **High Energy Density Nanoelectrofuel Flow Batteries for Transportation and Renewables: Development, Prospective and Challenges**
Carlo Segre (Duchossois Leadership Professor of Physics and Director of the Center for Synchrotron Radiation Research and Instrumentation, Illinois Institute of Technology), *E. V. Timofeeva, , J. P. Katsoudas1, V. K. Ramani, E. Moazzen, Y. Ding, S. Aryal, N. M. Beaver, Y. Li* (Illinois Institute of Technology), *S. Sen* (Argonne National Laboratory)

Development of transformational electrochemical energy storage technologies is an imperative for enabling sustainable technologies such as vehicle electrification and renewable energy generation. New approaches to battery materials, cell designs, and manufacturing offers fertile ground for scientific exploration across many disciplines, and promises to revolutionize the practice of energy storage.

We have developed a novel rechargeable nanoelectrofuel (NEF) flow battery technology, which leverages the properties of conventional solid state batteries, flow batteries and nanofluid technology. NEFs are stable dispersions of battery active nanoparticles in electrolyte that effectively charge/discharge as they are pumped through custom-designed flow cell(s) and represent a high-energy-density rechargeable, renewable, and recyclable electrochemical fuel. Nanoelectrofuels have high concentrations of active materials and exhibit liquid behavior in a wide range of temperatures for good flow and pump performance. NEF technology allows increasing the system level energy density of flow batteries to and above that of solid-state lithium-ion batteries. More than 50% improvement in energy density of solid batteries with the same chemistry are possible because of lower fraction of inactive packing material that is used in NEF flow battery.

The presentation will highlight the development of NEF flow battery prototype, which is scalable for electric vehicle needs, including engineering challenges in the development of NEF electrodes and electrochemical flow reactors and the approaches that we are using to solve them. Results of computational fluid dynamic (CFD) and electrochemical modeling will be presented and compared to empirical estimations. The utilization of these results in the context of an end product development will be discussed.

High energy density, pumpability and low cost of this cutting-edge innovation make it a good choice for numerous interchangeable industrial design applications, particularly for transportation and as an efficient way to store and distribution of energy from renewable sources. This presentation will also discuss technology transfer and commercialization challenges, potential development routes for NEF flow battery, including manufacturing and product development in the context of the present players, market size, and the long term vision for the technology.

Thursday Plenary Session I

Thursday, March 3, 2016 (Ballroom)

12:45 PM **Plenary Introduction**
Harold Kung (Northwestern University)

12:55 PM **Mechanistic Modeling of the (Bio)Conversion of (Bio)Macromolecules**
Linda Broadbelt (Sarah Rebecca Roland Professor and Chair, Department of Chemical and Biological Engineering, Northwestern University)

Fast pyrolysis, a potential strategy for the production of transportation fuels from biomass, involves a complex network of competing reactions, which result in the formation of bio-oil, non-condensable gaseous species, and solid char. Bio-oil is a mixture of anhydro sugars, furan derivatives, and oxygenated aromatic and low molecular weight (LMW) compounds. Previously, the successful modeling of fast pyrolysis reactors for biomass conversion was hampered by lumped kinetic models, which fail to predict the bio-oil composition. Hence, a fundamental understanding of the chemistry and kinetics of biomass pyrolysis is important to evaluate the effects of process parameters like temperature, residence time and pressure on the composition of bio-oil. In this talk, a mechanistic model that was recently developed to characterize the primary products of fast pyrolysis of cellulose is described. The kinetic model of pyrolysis of pure cellulose was then extended to describe cellulose decomposition in the presence of sodium salts. To quantify the effect of sodium, a density functional theory study of glucose dehydration, an important class of decomposition reactions of a cellulose-derived intermediate, was carried out. The theoretical results reveal alterations in the reaction rate coefficients when sodium is present and a change in the relative rates of different reactions. These kinetic parameters were used in the kinetic model to describe Na-mediated pathways, capturing trends in the experimental product distributions as the salt loading was increased based on classic catalytic cycles. In contrast to pyrolysis, conversion of macromolecules such as cellulose in Nature takes place at ambient temperature, aided by enzymes. Mechanistic details of the action of these enzymes will also be discussed and contrasted to high-temperature pyrolysis pathways.

We have also developed a computational discovery platform for identifying and analyzing novel biochemical pathways to target chemicals. Automated network generation that defines and implements the chemistry of what we have coined “generalized enzyme functions” based on knowledge compiled in existing biochemical databases is employed. The output is a set of compounds and the pathways connecting them, both known and novel. To identify the most promising of the thousands of different pathways generated, we link the automated network generation algorithms with pathway evaluation tools. The simplest screening metrics to rank pathways are pathway length and number of known reactions. More sophisticated screening tools include thermodynamic feasibility and potential of known enzymes for carrying out novel reactions. Our method for automated generation of pathways creates novel compounds and pathways that have not been reported in biochemical or chemical databases. Thus, our method goes beyond a survey of existing compounds and reactions and provides an alternative to the conventional approaches practiced to develop novel biochemical processes that harness the power of enzymes as catalysts.

Thursday Plenary Session II

Thursday, March 3, 2016 (Armour Dining)

12:45 PM **Plenary Introduction**
Brenton L. Cox (Exponent Inc.)

12:55 PM **CCPS Vision 20/20 --- A Call To Action**
Shakeel Kadri (Executive Director, AIChE Center for Chemical Process Safety)

Process safety is important to our individual health, to our company’s success, and to our region’s business economy. Companies that handle toxic, flammable, and explosive materials understand the importance of process safety and risk management. So do regulators. So should the community and other stakeholders. Individually these stakeholders have been working for years to improve process safety performance, however accidents continue to occur. It’s time to leverage our resources, knowledge and skills to all strive for a common goal of great process safety performance.

The purpose of this paper is to share CCPS’s Vision 20/20 with the Process Safety practitioners, business, engineering and operations leaders to begin the process of engaging the broader community in the vision with the spirit of “responsible collaboration” and the steps to achieve it. Vision 20/20 looks into the not-too-distant future to describe how great process safety is delivered when it is collectively and fervently supported by industry, regulators, academia, and the community worldwide. The paper will describes the characteristics of the best in class companies who have excelled in process safety. It identifies societal themes that are critical for the industry to achieve great process safety performance. It also reviews tools and resources that are available from CCPS for companies to evaluate their performance and take action to improve where needed.

Thursday Dinner and Dinner Keynote

Thursday, March 3, 2016 (Ballroom)

6:30 PM **Dinner**

7:15 PM **Local Section Announcments**
Adam Kanyuh (UOP/Honeywell)

7:25 PM **Keynote Introduction**
Georgia Papavasiliou (Illinois Institute of Technology)

7:30 PM **Materials and Protein Engineering for Modulating the Immune System**
Jeffery Hubbell (Barry L. MacLean Professor of Molecular Engineering Innovation and Enterprise, Institute for Molecular Engineering, University of Chicago)

Adaptive immune responses are triggered particularly powerfully in the lymph nodes and in the lymphoid tissues associated with mucosae. We are developing nanomaterials to exploit interstitial flow from the site of administration to the lymph nodes, using the nanomaterials to carry both antigen and adjuvant biomolecules. We are particularly interested in therapeutic vaccination in cancer, and we have determined that the tumor-draining lymph node is a particularly opportune lymphoid target for cancer vaccination. We are exploiting nanoparticles formed by emulsion polymerization and formed by self-assembly from block polymer amphiphiles and water soluble polymers as these delivery vehicles for both antigen and adjuvant molecules, creating multifunctional platforms that can be adapted to a wide variety of antigens.

In addition to inducing adaptive immune responses, so-called inverse vaccination to induce antigen-specific tolerance is of high interest. We are exploring biological and polymer approaches to deliver protein antigens in a tolerogenic manner, including targeting antigen to the surfaces of erythrocytes after injection, based on the premise that aged erythrocytes are cleared tolerogenically, along with exogenous antigen cargo they may carry. We have shown the ability to induce antigen-specific anergy as well as T regulatory responses, working in models of autoimmunity and of immune response to protein drugs. The liver is a target of particular interest, and we are developing polymers that can target antigen, tolerogenically, to particular cell populations in the liver.

Friday Morning Keynote Session

Friday, March 4, 2016 (Ballroom)

8:15 AM **Recognition for Volunteers from the GAC Chair**
Patrick Shannon (Middough Inc.)

8:25 AM **Keynote Introduction**
Paul Kenis (University of Illinois at Urbana-Champaign)

8:30 AM **Energy Infrastructure, Distribution & Trading: Ensuring That Supply Finds Demand**
Corey Correnti (Senior Vice-President, BP, retired 2015)

The rapid evolution of the U.S. energy industry, both in new technologies and available resources, is creating mismatches between supply and demand. Advances in new technologies have significantly changed the energy production landscape as well as the energy demand profile. Resource plays of varying qualities can be more remote from refining centers and consumer demand. New infrastructure is required to better connect these mismatches. However, these mismatches are difficult to forecast and require more dynamic trading and distribution capabilities to ensure that supply finds demand. This talk will explore the emerging trends in industry supply/demand (primarily crude oil through to transportation fuels) and the potential implications for energy distribution and trading going forward.

<u>Friday Plenary Session I</u>

Friday, March 4, 2016 (Ballroom)

12:45 PM **Plenary Introduction**

Carl Laird (Purdue University)

12:50 PM **Multi-scale Optimization for Chemical Processes**

Lorenz T. Biegler (Bayer University Professor and Head, Department of Chemical Engineering, Carnegie Mellon University)

Efficient Nonlinear Programming (NLP) algorithms and modeling platforms have led to powerful process optimization strategies. Nevertheless, these algorithms are challenged by recent evolution and deployment of multi-scale models (such as molecular dynamics and complex fluid flow) that apply over broad time and length scales. Integrated optimization of these models requires accurate and efficient reduced models (RMs). This talk presents a rigorous multi-scale optimization framework that substitutes RMs for complex original detailed models (ODMs) and guarantees convergence to the original optimization problem.

Based on trust region concepts this framework leads to NLP algorithms for RM-based optimization that deal directly with multi-physics models. The basic approach stems from a classical gradient-based trust-region method that includes multi-physics models. This algorithm is then extended through a DFO framework so that gradient calculations from the ODM can be avoided. We illustrate these algorithms with small examples and discuss RM-based optimization case studies on chemical processes and power plants, in order to demonstrate their performance and effectiveness.

<u>Friday Plenary Session II</u>

Friday, March 4, 2016 (Armour Dining)

12:45 PM **Plenary Introduction**

Zoltan Nagy (Purdue University)

12:50 PM **Continuous Processing in the Pharmaceutical Industry: Challenges and Opportunities**

Christopher Burcham (Eli Lilly & Co.)

Active pharmaceutical ingredients have historically been produced using batch manufacturing processes. Over the last decade, initiatives by regulatory agencies as well as efficiency drivers have focused the pharmaceutical industry to consider continuous processing in the development of manufacturing processes for innovative compounds in clinical development. Utilization of flow chemistry has afforded opportunities to implement continuous crystallization in drug substance manufacturing. The small lot sizes, purity, and control of physical properties (particle size and shape), create unique challenges in developing a continuous crystallization processes. However, with these challenges comes opportunity. Both the challenges and advantages of continuous crystallization will be presented in this talk.

<u>Friday Plenary Session III</u>

Friday, March 4, 2016 (Alumni Lounge)

1:55 PM **Plenary Introduction**

Marty Duran (BP)

2:00 PM **Reactor Internals for Hydroprocessing Units**

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

The catalyst companies are continuously developing more active catalyst to meet more stringent product specifications. In order to fully utilize today's catalyst technology it is imperative that the hardware is upgraded as well. Many of today's hydroprocessing units are using reactor internals designed 30+ years ago. Furthermore the feeds are different and the feed rate is most likely higher compared to the initial design, making it necessary to utilize new and properly designed, distribution trays, mixing chambers and scale catchers. The presentation will also highlight how improved safety for the people working with the trays have been included in today's optimized design.

<u>Closing Keynote and Reception</u>

Friday, March 4, 2016 (Ballroom)

5:45 PM **Invitation to MRC 2017**

Donald J. Chmielewski (Illinois Institute of Technology)

5:55 PM **Keynote Introduction**

Sohail Murad (Illinois Institute of Technology)

6:00 PM **Sustainable Change Management**

Manu Vora (Chairman and President, Business Excellence, Inc.)

In a world of constant change and an uncertain economy, Sustainable Change Management offers unlimited opportunities to create excellence and a competitive advantage. In today's turbulent environment, change can be used to your advantage. Dr. Vora will share core practices, giving you change management tools, concepts, and processes that are so vital for succeeding in today's complex world.

Join us for this inspiring presentation where you will discover the latest trends and best practices in Sustainable Change Management to achieve excellence! Learn how to apply change management in a variety of organizational situations and important initiatives. You will learn how great organizations sustain change. Tap into inspiring strategies, tools, and best practices that lead to success.

Presentation Abstracts

Biofuels I
Thursday, March 3, 2016 (Ballroom, **ThA1**)
Chair: *Ignasi Palou-Rivera* (LanzaTech)
Co-Chair: *Jill Jensen* (UOP/Honeywell)

9:45 AM **Low Temperature Hydrogenation of Pyrolytic Lignin over Ru/TiO2: 2D HSQC and 13C NMR Study of Reactants and Products** (ThA1a)

Daniel J. McClelland, Wen Chen, Ali Azarpira, John Ralph, George W. Huber (University of Wisconsin Madison), *Zhongyang Luo* (Zhejiang University)

Pyrolysis is a process for converting solid biomass into a liquid hydrocarbon feedstock. The resulting liquid, pyrolysis oil, is a complex mixture of more than 300 compounds. The pyrolysis oil is an emulsion that has a high oxygen content (50 wt%) and undergoes phase separation when heated for long period of time. Further catalytic upgrading of pyrolysis oil is necessary for producing fungible liquid fuels and chemicals though a major challenge of the upgrading process is the coke yields that deactivate the catalyst and plug the reactor. A large fraction of the coke formation is from the pyrolytic lignin fraction of the pyrolysis oil. The pyrolytic lignin fraction of the pyrolysis oil comes from the lignin portion of the biomass. Research into understanding the chemistry that occurs during the upgrading of this fraction is necessary in utilizing pyrolysis as a means for producing fuels and chemicals from biomass.

In this study, pyrolytic lignin and hydrogenation pyrolytic lignin were characterized by 2D 1H–13C HSQC and quantitative 13C NMR techniques. The pyrolytic lignin was produced from a mixed maple wood feedstock and separated from the bio-oil by water extraction. p-Hydroxyphenyl (H), guaiacyl (G), and syringyl (S) aromatics were the basic units of pyrolytic lignin while the native lignin β-aryl ether, phenylcoumaran, and resinol structures were not present. Hydrogenation was able to be carried out over a Ru/TiO2 catalyst at temperatures as low as 25 °C although coke formation was still present. A single-step hydrogenation at 150 °C reduced aromatic carbons by 40% and a three-step process reduced aromatic carbons by 74%. This demonstrates that it is possible to hydrogenate the pyrolytic lignin at low temperatures. A major challenge still to overcome is the coke formation during hydrogenation. The coke yield increased with hydrogenation temperature and decreased with the second and third steps of the three-step hydrogenation. When fractionating the pyrolytic lignin into low molecular weight (LMW) and high molecular weight (HMW) fractions, the HMW fraction hydrogenation yielded twice as much coke as hydrogenation of the LMW fraction.

References:

W. Chen, D. J. McClelland, A. Azarpira, J. Ralph, Z. Luo and G. W. Huber, Green Chem, 2015.

10:05 AM **Pilot Scale Demonstration of Green Gasoline Production from Woody Biomass** (ThA1b)

Naomi Klinghoffer, Rick Knight, Terry Marker, Jim Wangerow, Pedro Oritz-Toral, Martin Linck, Dan Swanson (Gas Technology Institute)

With growing interest in utilization of renewable and domestic energy sources, biomass has the potential to be a valuable feedstock for liquid fuels production, if it can be converted to liquid fuels in an economical manner. This presentation will discuss two approaches to producing transportation fuels from biomass. The IH2 process, an integrated hydropyrolysis and hydroconversion process, produces a liquid fuel with a yield of 80 gallons of gasoline per tonne of biomass, at a cost of ~$2.25/gallon. This process operates at moderate pressures of 350-500 psi and slightly lower temperatures than conventional pyrolysis processes, and has been demonstrated in a 50 kg/d continuous pilot plant. The TIGAS process encompasses an integrated biorefinery, which includes a biomass gasifier, tar reformer, acid gas removal, and gasoline synthesis. This process has been demonstrated at a pilot plant, which processes 21 tons of wood pellet feed per day, producing 23 barrels per day of gasoline product. The resulting fuel has been validated for EPA emissions and track-tested for 75,000 miles with no adverse findings. In addition, the potential of co-processing biomass and natural gas was studied for improving plant economics and reliability. We show that integration of non-catalytic partial oxidation of natural gas into a biomass-to-liquids process could lower production costs by 15%.

10:25 AM **Selective Hydrogenolysis of Glycerol into 1,3-propanediol via Highly Crystalline and Mesoporous WO3-Supported Ultrafine Pt Nanocrystals** (ThA1c)

Kai-Chieh Tsao, Yung-Tin Pan, Hong Yang, (University of Illinois at Urbana-Champaign), *Baoliang Lv* (Chinese Academy of Sciences)

Due to the fast depletion of the fossil fuels, using renewable resources such as biomass as the alternative energy has drawn tremendous attentions recently. Specifically, glycerol has been identified by the US Department of Energy as one of the top-12 building block which can be derived from biomass and be converted into value-added chemicals through a series of conversion processes. Among them, selective hydrogenolysis of glycerol into 1,3-propanediol (1,3-PDO) over 1,2-propanediol (1,2-PDO) has gained significant interest since the former can be used as the raw material for the production of various polyesters, polycarbonates and polyurethanes, and Pt/WO3 has been reported to be a candidate catalyst for the high selectivity.

Here we presented a simple template- and surfactant-free synthesis of highly crystalline mesoporous WO3 nanowire

bundles with polar (001) facet exposed, and the ordered nano-sized channels also help to generate ultrasmall and well-dispersed Pt nanocystals on the WO3 support because of the size confinement effect. The as-made Pt/WO3 showed high 1,3-PDO yield and 1,3-PDO/1,2-PDO selectivity, which can be attributed to the increased interface between Pt nanoparticle and WO3, with Pt metal and WO3 support responsible for H2 dissociation and anchoring the terminal hydroxyl group of the glycerol molecule, respectively. The inherent oxygen-deficient characteristic of the synthesized WO3 may also facilitate the adsorption of hydroxyl group on the oxygen vacant sites. We also demonstrated that the conversion to 1,3-PDO can be further improved by tailoring the WO3 nanostructure by carefully controlling the pH of the precursor solutions and the reaction time.

10:45 AM **The Influence of Catalysts on Biofuel LCA** (ThA1d)
Pahola Thathiana Benavides, Donald C. Cronauer, Jennifer B. Dunn (Argonne National Laboratory)

Biofuels are considered to be an important alternative to reduce the demand of fuels derived from conventional sources like petroleum, coal and natural gas. They provide environmental benefits over conventional fossil fuel such as the reduction of greenhouse gas (GHG) emissions which depend on the energy consumed in growing and harvesting the feedstock along with the energy consumed in converting the feedstock to the biofuel. These aspects are identified and measured by life cycle analysis (LCA) of the biofuel throughout its supply chain and end used. For some feedstock conversion processes, catalysts are critical inputs. Energy consumption and greenhouse gas (GHG) emissions during the production of catalysts and chemical inputs can influence biofuel life-cycle energy consumption and GHG emissions. This influence needs to be considered in biofuel life-cycle analysis (LCA). In this work, LCAs (i.e. cradle-to-gate) of three relevant catalysts (Pt/ γ-Al2O3, Mo/Co/ γ-Al2O3, and ZSM-5) used in the production of biofuels are presented. We also present their impacts in the LCA of biofuels and discuss processes that recover important metals from the spent catalyst and how these processes can influence biofuel LCA.

11:05 AM **Extract Nitrogen-Containing Compounds in Biocrude Oil Converted from Wet Biowaste via Hydrothermal Liquefaction** (ThA1e)
Karalyn Scheppe, Zhenwei Wu, Wan-Ting Chen, Yuanhui Zhang, Ken Nair (University of Illinois at Urbana-Cahmpaign), *Wanyi Qian* (Stanford University)

This study demonstrates that water can serve as a green solvent to achieve denitrogenation of biocrude oil converted from wet biowaste via hydrothermal liquefaction (HTL). It was hypothesized that water could extract relatively polar chemicals, such as nitrogen-containing compounds, in HTL biocrude oil. This hypothesis was examined by applying water as a solvent to biocrude oil converted from swine manure (SW) and low-lipid algae via HTL. Water solubility of biocrude oil and product yields (water extract, biocrude oil, solid residue, aqueous and gas products) were measured. Compared to a single stage extraction, the nitrogen content of biocrude oil converted from SW decreased from 4.32% to 3.23% while the heating value remained comparable. GC-MS analyses demonstrated that water can extract nitrogen-containing compounds and separate fatty acid derivatives that originally distributed into biocrude oil, though the elemental analysis infers that the extractive denitrogenation with water seemed to be ineffective for algal biocrude. When an ultrasonic-assisted extraction with water was conducted, the nitrogen content in algal biocrude oil decreased from 6.83% to 5.48%. In addition, GC-MS analyses suggest that fatty acid derivatives may behave similarly to surfactants and help emulsify nitrogen-containing compounds into water.

Cancer Therapies

Thursday, March 3, 2016 (Armour Dining, **ThA2**)
Chair: *Tim Whitehead* (Michigan State University)
Co-Chair: *Nicholas E. Clay* (University of Illinois at Urbana-Champaign)

9:45 AM **PEGylating Fibronectin Inhibits Tumor Growth and Invasion in an In-Vitro Model** (ThA2a)
Xue Geng, Jialing Xiang, Nancy Karuri (Illinois Institute of Technology)

The migration of cancerous cells from the tumor microenvironment to normal tissue is a fundamental step in the lethality many cancers including breast cancer. Some major differences between the tumor microenvironment and that of normal mammary tissue are: (i) an abnormally high level of fibronectin (FN), an extracellular matrix (ECM) protein, and (ii) high levels of proteases that cleave ECM components including FN. FN proteolysis is essential for tumor cell migration and FN fragments increase protease activity. Engineering FN stability in the tumor microenvironment may inhibit tumor cell migration and may be used as a therapeutic approach for non-resectable tumors. We have synthesized a number of FN-polyethylene glycol (PEG) conjugates that are more proteolytically stable than native FN and that have varying degrees of proteolytic stability depending on PEGylation variables. By using soft agar colony assay, we show differences in MDA-MDB231 breast cancer cell growth in medium with native FN and PEGylated FN. Tumor aggregates formed by MDA-MDB231 breast cancer cell are less numerous and smaller in medium with 5kDa PEGylated FN than in medium with native FN. These studies will be used in future to delineate the link between FN stability and tumor growth and invasiveness in model environments.

10:05 AM **High-Throughput Conformational Epitope Mapping to Guide Design of Structure-Based Vaccines** (ThA2b)
Tim Whitehead (Michigan State University)

We have developed a novel method for rapid determination of fine conformational epitopes. This platform technology involves deep sequencing of yeast displayed antigen libraries. I will present determination of critical (and previously unknown) neutralizing epitopes for pertussis toxin and a breast cancer target. Further, I will discuss methodological improvements in throughput and cost needed to integrate epitope mapping upstream in antibodies candidate selection. Implications for structural vaccine design will be discussed.

10:25 AM **Functionalized Flexible Palladium Nanosheets as Patches for HepG2 Cancer Cells** (ThA2c)
Yung-Tin Pan, Cartney E. Smith, Kam Sang Kwok, Jinrong Chen, Hyunjoon Kong, Hong Yang (University of Illinois at Urbana-Champaign)

Flexible, charged Pd nanosheets were prepared by solution phases synthesis and post synthesis treatment using short chain thiolated carboxylic acids and amines. They could wrap conformally around amine or hydroxyl functionalized micron-sized silica spheres driven by electrostatic interactions. When incubation with HepG2 cells, positively charged cysteamine (CA) functionalized Pd nanosheets exhibited a much higher cytotoxicity, showing more than 80% cell death at 100 ppm compare to the 30% with the negatively charged 3-mecaptopropionic acid (MPA) functionalized nanosheets. Scanning electron microscope images showed that the negative sheets formed 3D aggregates on the cell surface while the positively charge sheets formed a smooth coating. The results show through surface functionalization, Pd nanosheets can be modified to interact differently with HepG2 cancerous cells, resulting in varied cytotoxicity.

10:45 AM **Controlled Release of Drug Using Image Contrast Enhancing Nanoparticles** (ThA2d)
Courtney Collins, Madison Taylor, Sara Haworth, ZhanQuan Shi, Zishu Cao, Yoonjee Park (University of Cincinnati)

Retinoblastoma is a cancer of the eye that almost exclusively affects young children, often leading to vision loss. Although there are currently many treatments for retinoblastoma, these methods fail to eradicate all vitreous seeds, which are tumor cells that float in the vitreous of the eye and allow for reoccurrence to manifest. Diseases of the eye are challenging to treat due to the delicacy of the eye's tissues, making it essential to develop a drug delivery method that minimizes trauma and releases drug in a controlled manner. The main objectives of this study are to develop targeted stable nanoparticles which can controlled-release drug by external triggers with image contrast enhancing abilities to quantify the amount of drug release. By creating gold-coated nanoparticles that target vitreous seeds and release therapeutic agents by laser and ultrasound stimulation while also enhancing image contrast to aid with diagnosis, these objectives can be met. Particle formulation has been optimized by altering lipid shell composition, in order to maximize the stability and the ability to be triggered. In addition, in vitro studies with retinal pigment epithelial cells have shown that targeted particles are non-toxic and effectively attach to cells.

11:05 AM **Matrix Stiffness and Interstitial Flow Regulate Breast Cancer Malignancy in a Tumor-Microenvironment-on-a-Chip (TMOC) System** (ThA2e)
Nicholas E. Clay, Min Kyung Lee, Hyunjoon Kong (University of Illinois at Urbana-Champaign), *Kyeonggon Shin, Bumsoo Han* (Purdue University)

Living cells are subject to and regulated by a complex, three dimensional extracellular microenvironment constituted with soluble factors, matrix, and biofluids. As such, extensive efforts were made to recapitulate extracellular microenvironment in vitro and use the resulting system for both fundamental and applied bioscience studies. However, there are still several challenges to overcome, such as the independent control of properties of and interstitial fluid flow in a 3D matrix. To this end, this study demonstrates that a tissue microenvironment-on-a-chip (TMOC) platform engineered to present controlled matrix stiffness with a minimal change in matrix permeability and fluid flow allows us to examine the individual and combined effects of matrix mechanics and interstitial fluids on cellular activities in a 3D environment. The matrix stiffness was reduced by incorporating non-reactive poly(ethylene glycol) into a collagen gel, while the interstitial fluid flow in a gel was created by exposing the cell-laden gel to microfluidic flow at physiologically relevant rate. With breast cancer cells cultured in the TMOC platform, we discovered that a gel elastic modulus of 0.2 kPa upregulates cellular expressions of estrogen receptor-alpha (ER-alpha) and integrin, as compared with the stiffer gel. In both gel systems, interstitial fluid flow upregulates E-cadherin expression. We propose that such a TMOC platform would be broadly useful to study and regulate the phenotypic activities of a wide array of cells including therapeutic stem cells as well as cancer cells.

Process Safety I

Thursday, March 3, 2016 (Alumni Lounge, **ThA3**)
Chair: *Peter Herena* (Baker Engineering and Risk Consultants, Inc.)
Co-Chair: Amy E. Theis (Fauske & Associates)

9:45 AM **PSM Auditing & Lessons Learned to Enhance Overall Business Performance** (ThA3a)
Robert J. Weber (PSRG)

This presentation highlights common pitfalls identified during PSM audits conducted between 2005-2015 over a variety of industries ranging from oil and gas to petrochemical and specialty chemicals. The purpose of this presentation is also to highlight findings from recent OSHA NEP inspections in the refining and chemical industry, and the latest on planned changes to OSHA PSM / EPA RMP regulations at the Federal level and potential challenges that industry may face in order to try to comply with them.

10:05 AM **Inherent Hazards related to Gas Turbine and Steam Turbine Systems in Chemical Processes** (ThA3b)
Stephen Garner, Brenton Cox, Mark Fecke (Exponent)

Gas and steam turbines are used in a wide range of industrial services, e.g., driving mechanical equipment such as pumps, compressors, and electrical generators in the agrochemical and petrochemical industries. To ensure that a gas or steam turbines operate safely, reliably, and with optimum performance, turbines are typically provided with a control system designed either by the OEM or according to the OEM's specification. The OEM-provided control systems will typically include complex and integrated subsystems such as (but not limited to): a graphic user interface, an engine management system (EMS or ECS), a safety related system (SRS), and a package control system (PCS) that may interface with a facilities' existing computerized control and PI systems. Any failure of the mechanical systems, electro-mechanical systems, or logic-based control systems of a gas or steam turbine can pose both safety and process risks to a chemical processes. Unfortunately, many chemical engineers are not familiar with the mechanical and/or thermodynamic operating principles of gas and steam turbines. This presentation will discuss the fundamental operation of both gas and steam turbines and, utilizing case studies, identify common turbine system failure modes and their associated risks to chemical processes.

10:25 AM **Impact of Culture Change on Mechanical Integrity for SIS** (ThA3c)
Murtaza Gandhi (Baker Risk Engineering and Risk Consultants, Inc.)

Maintenance and testing of SIS is an important part of the Safety Life Cycle defined by ISA84/IEC61511. The maintenance program for SIS varies across the industry and is dependent upon the available expertise, management support and the philosophy of Preventive Maintenance (PM) found at each individual site.

To improve the maintenance cycle and make it fully compliant with the applicable standard, and to change the mentality of maintenance and operational personnel from a fix it "when it breaks" mentality to one of work planning, scheduling, execution, documenting and analyzing mentality may require a change in culture to achieve the desired results. The results of culture change with leadership support from the top down and supervisory involvement from the bottom up, lasting improvements to equipment mechanical reliability as well as safety can be made. This paper will discuss some the potential shortfalls identified in the maintenance and testing cycle supported with case a study that will provide insight into culture changes that can be introduced to improve the overall maintenance cycle.

10:45 AM **Advancing Process Safety** (ThA3d)
Scott M. Wozniak (UOP/Honeywell)

A joint program of the members of American Fuel and Petrochemical Manufacturers (AFPM) and the American Petroleum Institute (API) to continuously improve process safety through enhanced information, communication and collaboration. The Advancing Process Safety Program Consists of the Following Programs:

- Process Safety Performance Indicators - ANSI/API 754 Tier 1 & Tier 2 Events
- Event Sharing - Database for sharing events, causal factors and learnings
- Hazard Identification - Documents include Process Safety Hazards, Resources and References (API, NFPA, OSHA, etc.) and Significant Industry Incidents housed on the Safety Portal
- Regional Networks - Facilitated plant level discussions between process safety peers
- Site Assessment - Assessment of process safety systems against industry- developed protocols by independent and credible 3rd party teams
- Focus Improvements - Process Safety Bulletins on key learnings

11:05 AM **Latest Developments in Facility Siting (API RP752/753)** (ThA3e)
Ryan Terry, Brian Fagala (PSRG)

This presentation will present how to conduct an effective API RP 752 and RP 753 Facility Siting Study in order to address permanent and temporary process plant buildings. It also covers industry lessons learned and best practices from conducting these studies over the last ten (10) years.

Electro-Chemical Processes I

Thursday, March 3, 2016 (Herman Lounge, **ThA4**)
Chair: *Heather Barkholtz* (Northern Illinois University)
Co-Chair: *Jonathan Kucharyson* (University of Michigan)

9:45 AM **An Ambient Temperature Molten Sodium-Vanadium Battery with Aqueous Flowing Catholyte** (ThA4a)
Caihong Liu, Leon Shaw (Illinois Institute of Technology)

In a recent study, we have developed a new concept of room temperature hybrid sodium-based flow batteries (HNFBs) which are composed of a molten Na anode, flowing catholyte, and a Na-β"-Al2O3 solid electrolyte as the separator. This promising hybrid flow battery possesses many unprecedented advantages due to its unique battery design. However, it needed more endeavor to make these advantages practical. In this study, we focus on the key factors that dictate the long-cycle performance of HNFBs with V4+/V5+ redox couple based aqueous catholyte. These factors include the surface functionalization of graphite felt electrodes for the flowing catholyte, cell operation temperature, and properties of the solid electrolyte membrane. These understandings provide guidelines for improvement in the cyclic performance and stability of HNFBs, especially for the Na-V hybrid flow battery with aqueous catholytes. We demonstrate that the Na-V HNFB can reach high storage capacity (~70% of the theoretical capacity) with good Coulombic efficiency (90% ± 1% in 2–30 cycles) and cyclic performance (>99% capacity retention for 30 cycles). It shows the potential of high capacity Na-V aqueous flow batteries with excellent capacity rention and long cycling life. This is also the first demonstration that Na-β”-Al2O3 solid electrolyte can be used with aqueous electrolyte at near room temperature for more than 30 cycles.

10:05 AM **High Performance OER Catalyst of AxByOz Oxidesn** (ThA4b)
Jaemin Kim, Pei-Chieh Shih, Kai-Chieh Tsao, Xi Yin, Hong Yang (University of Illinois at Urbana-Champaign)
Although tremendous efforts have been devoted to the development of new class of electrocatalysts toward water electrolysis, most are limited to those operating under neutral or alkaline conditions due to the intrinsic instability of the metal-based catalysts in acid media in the applied potential range. We found a new AxByOz-type electrocatalyst showed exceptionally highly durability and activity towards oxygen evolution reaction (OER) with low Tafel slope. The OER mass current density and long-term stability greatly surpassed the performance of gold standard RuO2 OER catalyst in acid media. Density functional theory (DFT) calculation shows that the band center energy has an important role for the high OER performance, suggesting further improvement of electrocatalytic performance is possible under acidic condition.

10:25 AM **The Origin of Electrochemical Activity of Cobalt Oxide Water Oxidation Catalytic Amorphous Thin Film** (ThA4c)
Gihan Kwon, Anil Mane, Alex B. Martinson, David M. Tiede (Argonne National Laboratory), *Hacksung Kim, Jonathan D. Emery* (Northwestern University)
To investigate the origin of electrochemical performance as function of structural evolution of cobalt oxide water oxidation catalyst films, we utilized pair distribution function/resonant Raman/X-ray emission/inelastic X-ray scattering techniques. In this presentation, we present results on investigation of amorphous cobalt oxide in-situ film growth, domain structure, and comparison to electrochemical activity. The results show that amorphous cobalt oxide catalyst films (CoPi and CoBi) grow from nucleating small domains limiting size which depends on the nature of oxyanion present in electrolyte. Correlations between domain structures with electrocatalytic activity were investigated by comparing the catalytic activities with CoPi and CoBi films with various degrees of stacking. In addition, the electrical conductivity was directly measured using free standing cobalt oxide hollow tubes. The level of catalytic activity was found to correlate with film conductivity, number of catalytic sites, domain size, and degree of stacking. Charge can easily travel (delocalized) at intra-domain resulting from inelastic X-ray scatting but can’t easily travel at inter-domain resulting from low conductivity which was dominated by resistance between domains. We concluded that the resistance at inter-domain limits electrochemical activity of cobalt oxide catalyst films.

10:45 AM **Investigation of Oxygen Generation During Li-ion Battery Operation Using In-situ Fluorescence Spectroscopy** (ThA4d)
Mo Li, Javier Parrondo, Vijay Ramani (Illinois Institute of Technology)
An in-situ fluorescence spectroscopy system has been set up to study the interaction of selected fluorescent dyes (incorporated within the Li-ion battery structure) with oxygen, which serves as the quencher for the dyes. The release of oxygen during the degradation of LiCoO2 cathode material will be in-directly monitored in-situ during Li-ion battery charge and discharge at different C-rates. At present, dyes such as 9,10-dimethylanthracene and 1-hexyl-3-methylimidazolium bis (trifluormethylsulfonyl)imide have been examined ex-situ in the Li-ion electrolyte solvent environment at room temperature. Stern-Volmer relationships have been obtained and fitted to correlate the quencher (oxygen) concentration to fluorescence intensity. We will utilize these correlations to study the rate of oxygen ingress into the Li-ion battery electrolyte during operation.

11:05 AM **Selective Electrochemical Detection of Ciprofloxacin with a Porous Nafion/Multi-Walled Carbon Nanotube Composite Film Electrode** (ThA4e)
Pralay Gayen, Brian P. Chaplin (University of Illinois at Chicago)
We discuss the development of electrochemical sensors for the detection of Ciprofloxacin (CFX) in natural waters and wastewater effluents. The sensors are developed by depositing a layer of multi-walled carbon nanotubes (MWCNTs) dispersed in a porous Nafion film on to a boron-doped diamond (BDD) electrode substrate. The porous-Nafion-MWCNT/BDD electrode enhanced detection of CFX due to selective adsorption, which was accomplished by a combination of electrostatic attraction at –SO3- sites in the porous Nafion film, and the formation of charge assisted hydrogen bonding between CFX and -COOH MWCNT surface functional groups. By contrast, the bare BDD electrode did not detect CFX. The sensors were selective for CFX detection in the presence of other antibiotics (i.e., amoxicillin) and other non-target water constituents (i.e., Cl-, Ca2+, humic acid, sodium dodecylbenzenesulfonate, salicylic acid, 4-aminobenzoic acid, and 4-hydroxybenzoic acid). Differential pulse voltammetry obtained a limit of detection of 5 nM (S/N = 5) in a 0.1 M KH2PO4 supporting electrolyte (pH = 4.5). The linear range of current response with respect to CFX concentration was 0.05-10 μM, and the sensitivity was on the order of 2.07 μA μM-1. Although fouling of the sensor was observed at a high concentration of organic compounds (1 mM 4-aminobenzoic acid and 4-hydroxybenzoic acid), a short cathodic treatment could fully restore sensor performance. Results suggest that these sensors have applications in detecting CFX in natural waters and wastewater effluents.

Process Design and Optimization I
Thursday, March 3, 2016 (Crown Room, **ThA5**)
Chair: Juan Salazar (UOP/Honeywell)
Co-Chair: Mustafa Cagdas *Ozturk* (Illinois Institute of Technology)

9:45 AM **A Multi-Objective Optimization Approach to Optimal Sensor Location Problem in IGCC Power Plants** (ThA5a)
Pallabi Sen, Kinnar Sen (University of Illinois at Chicago), Dr. Urmila Diwekar (Vishwamitra Research Institute)
In order to operate an IGCC power plant in a safe and stable manner, many input and output process parameters need to be monitored. However, due to economic and operational constraints it is infeasible to place sensors at locations pertaining to all of these parameters. Hence, it becomes important to select the most effective sensor locations which can lead us to gain maximum information about the plant conditions. Drawing on the work done by "Lee & Diwekar", this paper attempts to broaden the realm of the optimal sensor location problem to address simultaneous optimization of multiple objective functions. In addition to "Fisher Information", two other objective functions, viz., "thermal efficiency of the power plant" and "cost", will be considered. Practical issues present in an IGCC power plant such as harsh physical conditions and variability in process parameters make the optimal sensor location problem an especially complicated one. Advanced simulation software and data from a set of existent sensors are used to collect information about the output parameters which do not have any sensors to gauge them yet. In order to solve this real world large scale problem, we use a novel algorithm called Better Optimization of Nonlinear Uncertain Systems (BONUS). BONUS works in probability distribution space and avoids sampling for each optimization and derivative calculations iterations.

A non-linear stochastic multi-objective problem has been solved to determine the non-dominated or Pareto set which contains different options for optimal sensor network locations that can simultaneously satisfy the three objective functions, (maximizing observability, minimizing cost and maximizing the IGCC power plant thermal efficiency).

10:05 AM **Profit Based Sensor Network Design Revisited: Application of the Generalized Bender Decomposition** (ThA5b)
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).

10:25 AM **A Nonlinear Optimization Approach to the Estimation of Spatial Transmission Parameters in Infectious Disease Spread** (ThA5c)
Todd Zhen, Carl D. Laird (Purdue University)
Highly infectious pathogens can cause enormous outbreaks that are followed by regional extinction as it runs out of susceptible hosts. Rescue effects due to spatial transmission of these pathogens can once again spark epidemics and lead to regional persistence. In this work, we develop a framework for efficient estimation of city-to-city spatial transmission rates by inferring transport information from localized disease case data. The model is formulated with nonlinear constraints, giving a nonlinear programming problem that is solved using an interior-point solver. We first estimate the strength of city-to-metapopulation spatial transmission using disease fade-out information between outbreaks, and, second, extend the model to estimate the strength of city-to-city spatial transmission. The estimation is demonstrated using records of measles outbreaks in 954 cities across England and Wales between 1944 and 1964. We find that our approach is very feasible for this large-scale estimation, and accurately reproduces literature values. Additionally, our approach for estimating disease transmission parameters is flexible, and allows for further investigation of larger model spaces.

10:45 AM **An Efficient Superstructure Generation and Modeling Framework** (ThA5d)
WenZhao (Tony) Wu, Carlos A. Henao, Christos T. Maravelias (University of Wisconsin Madison)
One of the fundamental problems in chemical engineering is the synthesis of a process, that is, to select unit operations,

their interconnections and operational conditions to create a flowsheet that meets process constraints and requirements, aiming at technical, economic and/or environmental optimality. Superstructure optimization is a powerful approach to solving the process synthesis problem. In this work, we develop an efficient superstructure generation and modeling framework. For superstructure generation, we develop a new way of superstructure representation using three elements-units, unit ports and general conditioning streams, as well as four connectivity rules based on “minimal” and “feasible” component sets to generate the simplest superstructure containing all feasible processes. For superstructure modeling, we develop a modular modeling approach and present a complete general superstructure model and its MINLP reformulation, which are designed to work coherently with our proposed generation method. The proposed framework provides a complete procedure for superstructure generation followed by modeling, allowing efficient model creation, modification and code recycling.

11:05 AM **Novel Sampling Technique for High Dimensional Stochastic Optimization Problem** (ThA5e)
Nishant Dige, Urmila Diwekar (University of Illinois at Chicago)

Uncertainty is essence of real world optimization problem. Computational speed is critical in optimizing large scale stochastic problems. The major bottleneck in solving large scale stochastic optimization/stochastic programming problems is the computational intensity of scenarios or samples. To this end, this paper presents a novel sampling approach. There are two important properties for sampling randomness and uniformity. It is the uniformity that is important for accuracy of the sampling. Latin Hypercube sampling (LHS) provide good convergence rate as compared to random Monte Carlo simulations but LHS shows uniformity in single dimension only. For Multi Dimension it computes stratified sampling for each uncertainty but randomly pairs to form a K dimensional sample set. Due to this random combination; good uniformity for single dimension is lost for K dimension. Furthermore quasi random sequences like Hammersley, sobol, and Halton sequences show better uniformity in k-dimensions but are not one dimensionally uniform. For Quasi Monte Carlo sequence sampling pairings are done as per Hammersley or Sobol sequence points to form a sample set of K dimension. For higher dimension (more than 40) some of these quasi-random sequences like Hammersley and Halton show clustering/pattern effect due to exponential increase in prime base. Sobol sequence sampling is not linked to the prime base so for dimension more than 40 there are no clustering effect and uniformity is achieved. Computing LHS sampling and pairing them using Sobol sequence sampling provided better uniformity in one dimension as well as K dimension. Therefore, in this paper we are deriving this new sampling technique by combining one dimensional uniformity of LHS and k-dimensional uniformity of Sobol. This novel sampling technique has higher computational convergence rate.

Keywords: Sampling, Quasi Sequence Sampling, Sobol Sampling, Optimization under uncertainty, stochastic supply chain network design

Biofuels II

Thursday, March 3, 2016 (Ballroom, **ThB1**)
Chair: *Eric Doskocil* (BP)
Co-chair: *Dan McClelland* (University of Wisconsin)

2:00 PM **Biocomposites for Algae Production** (ThB1a)
Omar Khalil, Reza Ghodsi, Bader Jarai, Fouad Teymour (Illinois Institute of Technology)

Biofuels derived from algae biomass have a promising outlook for becoming an important contributor to our future energy portfolio. Intensive research in underway nationally and internationally to improve the efficiency of this process and to overcome several obstacles that have been delaying the path to commercialization. Among those, the separation of algal biomass from its medium is of prime importance as it could be energy intensive, and is essential as the economics of the process mandate the reuse of the nutrient-rich medium.

We have solved this problem by growing the algae using a novel approach, the stabilized flocculated mode. To achieve this processing condition we induce flocculation by adding a bio-flocculant, namely a filamentous cyanobacterial organism. The bacteria has a natural tendency to entangle into nest-like networks that provide a suitable medium for the growth of the algae. Several factors govern the process of absorption of the algae onto the bacterial flocs and the symbiotic relation between them. We have studied the integration between the two organisms in detail and report on our experimental findings in this talk. The flocs are stabilized using shear resulting from aeration devices that both control the size of the flocs, deliver the necessary carbon dioxide, and control the oxygen concentration in the medium. The separation process is greatly simplified in this mode, as the cessation of aeration reverse the process and induces flocculation.

We also report on our efforts in the conversion of biomass to biofuel, where we attach importance to two crucial concepts: a) Total utilization of the biomass, and b) Direct transesterification of the oil prior to separation from the biomass. Preliminary experimental results have established the feasibility of achieving those.

2:20 PM **Techno-Economic and Environmental Life Cycle Assessments of Hydrocarbon Biofuel from Poplar** (ThB1b)
David Shonnard, Olumide Winjobi, Wen Zhou, Paul Langford, 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 rapid thermal degradation of wood in the absence of air at a temperature of approximately 500-550OC with a short residence time of less than 2 seconds.

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 size reduction. Torrefaction, often referred to as mild pyrolysis, tends to enhance bio-oil properties by reducing water content, minimizing acidity, and reducing size reduction energy. The impact different torrefaction temperatures has on the cost of production as well as the environment is being 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-based process. Effects of the use of renewable co-products such as char and non-condensible gases from pyrolysis to replace fossil energy inputs to the process are explored in scenario analysis.

Aspen Plus process simulation package is being used to model the two stage torrefaction-fast pyrolysis process with catalytic upgrading of pyrolysis bio-oil to hydrocarbon fuel blends. The effect of torrefaction severity on composition and yield of pyrolysis bio-oil is being included using data from the NSF-funded Sustainable Energy Pathways project at Michigan Tech based on micro- and pilot-scale pyrolysis and catalytic upgrading, while the work of Phanphanich et al (2011) [1] is being 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 and catalytic upgrading as a result of the torrefaction pretreatment step.

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

2:40 PM **Greenhouse Gas Emissions of Ethanol Production Via the LanzaTech Process from Biomass Cellulosic and Waste Gas Feedstocks** (ThB1c)

Ignasi Palou-Rivera (LanzaTech), *Robert Handler* (Michigan Technological University)

LanzaTech has developed a novel ethanol manufacturing process via gas fermentation of carbon-containing gases. In this study, a life-cycle assessment method is used to quantify the global warming potential of several scenarios for producing renewable ethanol with the LanzaTech process. The considered scenarios include ethanol produced from steel mill waste gases and from gasified cellulosic biomass. Using standardized life-cycle assessment methods, ethanol produced via LanzaTech fermentation shows greenhouse gas emissions that are beyond 60% lower than conventional fossil gasoline, with biomass-based ethanol achieving close to 90% emission reductions. Results indicate that the LanzaTech gas fermentation technology can be a viable alternative for producing next-generation renewable fuels with a reduced greenhouse gas emissions footprint contributing to the UN goal of limiting warming to 2 C and reducing our use and dependence on fossil fuels.

3:00 PM **Production of Transportation Fuels by Co-Processing Biomass-Derived Pyrolysis Oils in a Petroleum Refinery Fluid Catalytic Cracking Unit** (ThB1d)

Jill R. Jensen, Chad R. Huovie, Stanley J. Frey (UOP/Honeywell)

Honeywell's UOP has made substantial progress in making the production of low-capital investment cellulosic transportation fuel a reality using Ensyn's biomass-derived RTP green fuel as feedstock. The concept is to convert the RTP green fuel, produced by pyrolysis of cellulosic biomass, in an existing petroleum refinery's fluid catalytic cracking (FCC) unit to produce incremental gasoline and diesel. UOP has developed methods of addition, established principles of operation, and evaluated the effects of RTP green fuel in an FCC unit and impacts downstream in the refinery. This work and resulting technology enables FCC operators to confidently include RTP green fuel with their petroleum feedstock without negative effects to equipment reliability, product quality, and integration with the overall refinery. A review of impacts of co-processing pyrolysis oils on the various FCC product stream yields and quality will be discussed along with the work that has been completed to mitigate risks to ensure smooth and reliable operation in the refinery.

3:20 PM **Upgradation of Biocrude Oil Converted from Bio-Wastes via Hydrothermal Liquefaction into Drop-in Fuel and Value-Added Chemicals** (ThB1e)

Wan-Ting Chen, Yuanhui Zhang, Peng Zhang (University of Illinois at Urbana-Champaign)*, Lance Schideman, B.K. Sharma* (Illinois Sustainability Technology Center)

Biorefineries of biocrude oil products converted from wet biowastes such as swine manure and algae via hydrothermal liquefaction (HTL) are in need of a comprehensive understanding. The goal of this study is to develop multi-phase bio-refineries to expedite the downstream application of biocrude oil into drop-in transportation fuels and value added chemicals, such as nitrogen-doped hydrocarbon electric materials. Our previous study showed that biocrude converted from wet biowaste, such as swine manure, food waste, and mixed-culture algae from wastewater via HTL, contain appreciable higher heating values (HHV) ranging 32-38 MJ/kg, while the HHV of ethanol and gasoline are respectively about 29 MJ/kg and 45 MJ/kg. However, the relatively high concentration of impurities in the biocrude oil, mainly nitrogen (3-7%), oxygen (about 10%) and moisture content (up to 20%), remain problematic that needs to be addressed in order to utilize this source as transportation fuels. As a consequence, further upgrading or separation of the biocrude oil products is critically needed. Several previous studies have demonstrated that catalysts (e.g. zeolites, Pt/C, Raney-Ni, Rh etc.) have little impact on upgrading the biocrude oil when the reaction temperature was below 500 °C. On the contrary, it was reported that after proper separation, such as distillation, the oxygen content in the biocrude oil could be reduced to 5% and the heating values could be increased up to 41-45 MJ/kg, which indicates that there is a high potential to utilize these biocrude oil products as drop-in fuels. This study aims to utilize a pilot scale plug-flow reactor to produce 8-10 gallons of biocrude oil and separate biocrude oil products into drop-in transportation fuels and value-added chemicals with distillation. Preliminary study shows that about 60% of the biocurde product can be distilled out before 250 °C. Distillation curve is also recorded and will be compared to that of jet fuel, diesel and lubricant oil. Elemental and GC-MS analyses demonstrates that the distillate fractions collected between 200-250 °C have similar chemical properties to diesel. Heating values and densities of distillate products were also measured. The non-distillable products were also examined in terms of elemental compositions and SEM microscopy. Physiochemical characterization suggests that the non-distillable products may serve as carbon-based adsorbents or nitrogen-doped electrical capacitors.

Drug Delivery I

Thursday, March 3, 2016 (Armour Dining, **ThB2**)
Chair: *Haipeng Lui* (Wayne State University)
Co-chair: *Benjamin M King* (University of Iowa)

2:00 PM **Exploring the Possibility of Exploiting Protein Corona for Targeted Nanoparticle Delivery** (ThB2a)
Vahid Mirshafiee, Raehyun Kim, Soyun Park, Mary L. Kraft (University of Illinois at Urbana-Champaign), *Morteza Mahmoudi* (Stanford University)

Nanoparticles (NPs) are routinely functionalized with targeting ligands (e.g. antibodies) to enable their selective delivery to the desired site in the human body, and enhance their uptake by target cells. However, upon introduction of functionalized NPs to the blood stream, plasma proteins bind to their surfaces and form a protein layer, named “protein corona,” that would cover the targeting ligands and reduce the targeting capabilities of functionalized NPs. In order to address this challenge, we aimed to explore the possibility of directing the plasma protein adsorption onto NPs towards formation of a functional protein corona that has targeting capabilities and could be utilized for NP targeted delivery. Here, we used the well-studied opsonin-mediated phagocytosis of NPs to assess if protein corona could be exploited to stimulate NP uptake by desired cells. Our results demonstrated that pre-coating NPs with gamma globulins promoted the binding of immunoglobulins to the NPs upon incubation of pre-coated NPs with plasma proteins, and formed a protein corona enriched with opsonins. Despite enrichment of protein corona with opsonins, our cellular uptake analysis indicates that this opsonin enrichment did not increase NP uptake by macrophages. In fact, assessment of opsonins accessibility on NPs indicated that the opsonins in the corona were screened by other plasma proteins bound to the NPs. Thus, beside enrichment of protein corona with desired proteins that have natural targeting capabilities, it is important to control the spatial orientation and accessibility of these proteins in the corona in order to utilize the functional protein corona for targeted delivery applications.

2:20 PM **Effect of PEGylated Gold Nanoparticle Permeation on lipid bilayer membranes** (ThB2b)
Priyanka A. Oroskar, Cynthia Jameson (University of Illinois at Chicago), Sohail Murad (Illinois Institute of Technology)

In targeted drug delivery systems, nanoparticle carriers are often functionalized with polyethylene glycol (PEG) polymers to improve solubility and in-vivo stability in biological media. Gold nanoparticles decorated with ligands are excellent candidates in particular for delivery of therapeutic agents. This is due to their distinctive physical and chemical characteristics, which include the ability to be synthesized in a wide range of shapes and ease of functionalization of the nanoparticle surface. In this study, we have carried out a series of coarse-grained molecular dynamics simulations to investigate the permeation of polyethylene oxide (methyl-terminated PEG or PEO) functionalized gold spherical nanoparticles and nanorods across a protein free phospholipid bilayer membrane. Investigation of permeation of functionalized nanoparticles under various conditions is important because it can aid in developing strategies for using nanoparticle as drug carriers while suppressing cytotoxic effects as they permeate cell membranes in-vivo. Previously we have shown that ligand-coated gold nanoparticle permeation across lipid bilayer membranes induces water and ion penetration as well as incidence of lipid flip flop and lipid displacement.

In our studies we have studied the effect of ion concentration gradients, nanoparticle shapes, nanoparticle permeation velocities, length of PEO ligands, and chain density of grafted PEO ligands on water and ion leakage, lipid flip-flop, and lipid loss from the lipid bilayer membrane. Additionally, the mechanism of penetration of the PEO functionalized nanorods and spherical nanoparticles into the bilayer and the nature of the interactions between the PEO ligands and the lipids of the bilayer are discussed. The results of this work will be of interest to experimentalists who engineer nanoparticles with surface modifications for biomedical applications.

2:40 PM **Development of a Photoresponsive Scaffold Composed of Self-Assembled Nanostructures** (ThB2c)
Nicholas Karabin, Evan Scott (Northwestern University)

Stimuli responsive polymers can provide enhanced spatiotemporal control over the delivery and biodistribution of therapeutic payloads. Here, we describe the development of a novel, photoresponsive scaffold composed of self-assembled poly(ethylene glycol)-bl-poly(propylene sulfide) (PEG-bl-PPS) nanostructures. Depending on the molecular weight ratio of the hydrophilic PEG and hydrophobic PPS blocks, diverse nanostructures can be assembled, including solid core micelles, vesicular polymersomes, and high aspect ratio filomicelles [1]. Functionalization of the surfaces of the assembled nanostructures permitted their crosslinking into novel scaffolds capable of encapsulating and delivering hydrophilic, hydrophobic, and amphiphilic molecules. The oxidation sensitivity of PPS allows manipulation of the hydrophilic:hydrophobic ratio, and we therefore used photooxidation to transition from one morphology to another for controlled delivery. ROS-generating photooxidizers were stably loaded within the hydrophobic domains of PEG-bl-PPS structures to provide light-mediated changes in nanostructure morphology. Excitation of the photooxidizer triggers a cascade of reactions that culminates in the oxidation of PPS into the more hydrophilic poly(propylene sulfone) or poly(propylene sulfoxide) [2]. Consequently, this light-induced oxidation destabilized the scaffold into micellar structures, which can subsequently transport and target diverse payloads to specific cell populations. Our ability to tailor scaffold properties is demonstrated through rheological data obtained for scaffolds exhibiting varying crosslinking densities. Controlled photodestabilization is exhibited through a decrease in scaffold stability following irradiation, as well as through the delivery of model therapeutics.

[1]. Cerritelli, Simona, et al. "Aggregation Behavior of Poly (ethylene glycol-bl-propylene sulfide) Di-and Triblock Copolymers in Aqueous Solution." Langmuir 25.19 (2009): 11328-11335.
[2]. Vasdekis, Andreas E., et al. "Precision intracellular delivery based on optofluidic polymersome rupture." ACS Nano 6.9 (2012): 7850-7857.

3:00 PM **Polyphosphate loaded Nanoparticles for Suppression of Bacterial Collagenase and Intestinal Healing** (ThB2d)
Dylan Nichols, Fouad Teymour, Georgia Papavasiliou (Illinois Institute of Technology), *Melissa Arron, Olga Zaborina, John Alverdy* (University of Chicago)

The intestinal tract undergoes a variety of injuries both as a result of disease processes as well as from direct surgical manipulation. The process by which successful repair and return of function occurs following these injuries is dependent on the composition and function of the intestinal microbiota which can either enhance or disrupt the intestinal healing process. Previous studies have shown that under phosphate deprived conditions pathogenic intestinal microbes produce high levels of collagenase, a key phenotype involved in impaired healing in the intestinal tract. Common treatment approaches involve administration of antibiotics, which have been shown to disrupt the normal flora that is responsible for enhancing the healing process. To this end, we have focused on phosphate-based therapeutic compounds to selectively suppress pathogenic bacterial phenotypes. We have previously developed an approach for synthesizing polyphosphate (PPi) loaded nanoparticles (NPs) using inverse phase miniemulsion polymerization. The nanoparticles allow for sustained release of PPi and result in suppression of P. aeruginosa virulence in vitro in a dose-dependent manner while maintaining bacterial survival. Our recent data demonstrate that both free PPi, as well as PPi loaded NPs, are effective at suppressing collagenase of S. marcescens. Current efforts are aimed at testing the effectiveness of PPi loaded NPs in suppressing collagenase in a variety of gram positive and gram negative pathogens.

3:20 PM **Photo-Click Hydrogels Prepared from Functionalized Cyclodextrin and Poly(ethylene glycol) for Drug Delivery and In-Situ Cell Encapsulation** (ThB2e)
Han Shih, Chien-Chi Lin (Purdue University)

Polymers or hydrogels containing modified cyclodextrin (CD) are highly useful in drug delivery applications as CD is a cytocompatible amphiphilic molecule that can complex with a variety of hydrophobic drugs. Here, we designed modular photo-click thiol-ene hydrogels from derivatives of βCD and poly(ethylene glycol) (PEG), including βCD-allylether (βCD-AE), βCD-thiol (βCD-SH), PEG-thiol (PEGSH), and PEG-norbornene (PEGNB). Two types of CD-PEG hybrid hydrogels were prepared using radical-mediated thiol-ene photo-click reactions. Specifically, thiol-allylether hydrogels were formed by reacting multi-arm PEGSH and βCD-AE, and thiol-norbornene hydrogels were formed by cross-linking βCD-SH and multi-arm PEGNB. We characterized the properties of these two types of thiol-ene hydrogels, including gelation kinetics, gel fractions, hydrolytic stability, and cytocompatibility. Compared with thiol-allylether hydrogels, thiol-norbornene photo-click reaction formed hydrogels with faster gelation kinetics at equivalent macromer contents. Using curcumin, an anti-inflammatory and anti-cancer hydrophobic molecule, we demonstrated that CD-crosslinked PEG-based hydrogels, when compared with pure PEG-based hydrogels, afforded higher drug loading efficiency and prolonged delivery in vitro. Cytocompatibility of these CD-crosslinked hydrogels were evaluated by in situ encapsulation of radical sensitive pancreatic MIN6 β-cells. All formulations and crosslinking conditions tested were cytocompatible for cell encapsulation. Furthermore, hydrogels crosslinked by βCD-SH showed enhanced cell proliferation and insulin secretion as compared to gels crosslinked by either dithiothreitol (DTT) or βCD-AE, suggesting the profound impact of both macromer compositions and gelation chemistry on cell fate in chemically crosslinked hydrogels.

Process Safety II

Thursday, March 3, 2016 (Alumni Lounge, **ThB3**)
Chair: *Scott Wozniak* (UOP/Honeywell)
Co-chair: *Jesse Calderon* (Baker Engineering and Risk Consultants, Inc.)

2:00 PM **Five Steps to Managing Combustible Dust Hazards** (ThB3a)
Amy Theis (Fauske & Associates, LLC)

Combustible dust, under certain circumstances, has the potential to cause fires and explosions, which could lead to personnel injury or death, property damage and business interruption. A five step approach will be presented for managing combustible dust hazards at a facility. These steps include: 1) Characterizing dust hazards, 2) Performing a Dust Hazard Analysis (DHA), 3) Implementing fire/explosion protection systems based on DHA recommendations for risk reduction, 4) Developing and documenting combustible dust management systems for safety and compliance purposes, and 5) Conducting self-audits to maintain the combustible dust program/systems. Details and guidance will be provided for each of these steps including recommended combustible dust tests based on dust handling operations. Best practices for explosion protection strategies will be reviewed based on applicable standards, codes and regulations, e.g., National Fire Protection Association (NFPA). This will include documentation required for management systems such as housekeeping, training, managing process changes, inspection and maintenance. A process life cycle approach will be presented where these five steps are continuously utilized to ensure that equipment and management systems provide appropriate protection for potential fires and explosions due to combustible dust hazards.

2:20 PM **CFD Based Thermal Fatigue Risk Assessment in Refinery Process Lines** (ThB3b)
Raj Venuturumilli, Madhusuden Agrawal, Samir Khanna (BP)

Flow turbulence at the mixing points of process fluids can generate large temperature fluctuations. If these fluctuations are transmitted to the pipe walls then they will suffer thermal fatigue induced damage over time. Often special injection devices at the mixing points mitigate the temperature fluctuations. Computational Fluid Dynamic (CFD) methodology can be effectively used to predict and quantify the thermal fluctuations in the fluid as well as at the walls. An overview of the technique will be presented with the help of a few case studies.

2:40 PM **Extending the Life of a High Temperature Refinery Reactor** (ThB3c)
Jerry Wilks (CITGO Petroleum Inc.)

Lemont Refinery has a fluidized bed catalytic cracking reactor made of UNS K12062 steel that had operated for 38 years in the 510 535°C temperature range when it was discovered in 2006 that the vessel was approaching the end of its life. Inspections of the reactor conducted in 2008 revealed small cracks developing in several of the vessel welds. To arrest further cracking a new weld repair technique was tested: external reinforcement of the weld with UNS N06625 weld overlay. When the unit came down for a scheduled shut-down in 2010, those repairs were cut out and tested, and it was discovered that the weld overlay had stopped creep crack propagation. In 2012, additional creep cracking occurred in plates a few inches from welds. Analysis of the vessel determined that a large nozzle was creating high stresses in a zone beyond welds when the vessel was rapidly heated during start-ups. In order to extend the life of the vessel until it could be replaced, all the vertical seams in the vessel were weld overlaid with UNS N06625 in 2012. Also, process limits for the unit were changed to reduce damage to the reactor. Then on-line repairs were made following the repair guidelines in ASME PCC-2[1] to further extend the reactor life. This reactor was replaced in June of 2015. The repairs conducted had effectively extended the reactor's life about 10 years resulting in significant refinery savings.

3:00 PM **A Maturity Model for Assessing your Company's PSM Program** (ThB3d)
Madonna Breen (PSRG)

This presentation covers a 4 stage PSM maturity model and tool for assessing the health and wellbeing of your Company's PSM program.

3:20 PM **LOPA and the Art of Motorcycle Maintenance** (ThB3e)
Peter Herena (Baker Risk Engineering and Risk Consultants)

Layers of Protection Analysis (LOPA) is a frequently-used tool to provide a semi-quantitative estimate of risk. It is a more rigorous approach than the traditional Hazop, but less so than time-consuming and highly detailed Quantitative Risk Analysis (QRA). However, like any tool, it can be misapplied under certain conditions, which can lead to seemingly spurious results. In an environment of cost minimization, often process engineers or project managers are left to undertake LOPA with minimal training or guidance.

The presentation will discuss some “hot button” topics related to LOPA, and the kind of questions a project manager, process engineer or active team member should ask PRIOR to the meeting so that the outcome can be sensible and effective. Relevant recent updates to procedures and guidelines will be discussed so attendees can continue research on their own.

Electro-Chemical Processes II

Thursday, March 3, 2016 (Herman Lounge, **ThB4**)
Chair: *Gihan Kwon* (Argonne National Laboratory)
Co-chair: *Canan Acar* (University of Ontario Institute of Technology)

2:00 PM **Electrodeposition of Copper for Metamaterial Fabrication** (ThB4a)

Shendu Yang (University of Missouri)

Metamaterials, a class of artificial optically-active materials with exceptional properties based on their patterned structures, typically use metallic and dielectric repeating features to provide a negative index of refraction. In the fabrication of metamaterials utilized in this study, copper is selected for the metallic part of metamaterial due to its high thermal and electrical conductivity, excellent mechanical properties and relative ease of acquisition.

Electrodeposition from a highly-acidic copper electrolyte is the most attractive approach for fabricating the conductive component of the metamaterial in this study due to its ease of control and rate of deposition. However, since the presence of special high-aspect ratio design features in the metamaterial requires bottom-up superfilling and leveling of micron and sub-micron scale volumes; additives such as chloride ions, 3-mercapto-1-propanesulfonate (MPSA), polyethylene glycol (PEG), and polyvinylpyrrolidone (PVP) are introduced into the electrodeposition process in order to provide excellent conformality and adhesion. Most of the present study focuses on investigating the optimal parameters of electrodeposition of copper such as the concentration of each of the additives, the effects of additive aging, and the electrodeposition parameters of deposition voltage and its corresponding current density.

Electrochemical methods such as cyclic voltammetry and controlled potential coulometry probe the mechanism of both the specific effects of additives and the interplay between additives. In parallel, COMSOL finite element modeling (FEM) software is used to simulate the 2D electrodeposition of copper to investigate the mass transfer and the electrochemical behavior of the electrodeposition system.

Atomic force microscopy (AFM), four-point probe sheet-resistivity measurements, and optical microscopy are used as characterization tools to map the surface topography, sheet resistances, and surface roughness of the deposited films. Combined with the electrochemical methods, optimized parameters for electrodeposition of copper are obtained and desired fabrication methods for metamaterials are achieved in this study.

2:20 PM **Engineering Nanofluid Electrodes: Control of Rheology and Electrochemical Activity of Nickel Hydroxide Nanoparticles** (ThB4b)

Elahe Moazzen, Carlo Segre (Illinois Institute of Technology), *Sujat Sen, Chun Man Chow, Elena Timofeeva* (Argonne National Lab)

Nanofluid electrodes or nanoelectrofuels have significant potential in the field of flow batteries, as at high loadings of solid battery active nanoparticles, their energy density can be orders of magnitude higher than in traditional redox flow battery electrolytes. Requirements to nanofluid electrodes are that they must have a manageable viscosity at high particle concentrations (i.e. easily pumpable) and exhibit good electrochemical activity towards charge and discharge reactions. Engineering of such nanofluid electrodes involves development of new and unique approaches to stabilization of nanoparticle suspensions. In this work, we demonstrate a surface modification approach that allows controlling the viscosity of nanofluids at high solid loading, while simultaneously retaining electrochemical activity of nanoparticles. A scalable single step procedure for the surface grafting of small organic molecules onto nickel (II) hydroxide nanoparticles (Ni(OH)2) is demonstrated. Modified nickel hydroxide nanoparticles have a small amount (<3 wt. %) of the grafting moiety on the surface, which helps formulating stable dispersions with up to 60 wt. % of solid loading in alkali aqueous electrolytes with a maximum viscosity of 32 cP at room temperature. For comparison suspension with 5 wt. % of pristine nanoparticles shows viscosity of >2500 cP. Suspensions of surface modified Ni(OH)2 particles also show up to 60% enhancements in thermal conductivity, as compared to base electrolytes. Electrochemical testing of the pristine and modified nanomaterials in the form of solid casted electrodes showed reversible discharge capacities exceeding 250 mAh/g indicating comparable electrochemical activity of both samples close to the theoretical limit of 289 mAh/g.

2:40 PM **Characterization of Electronic and Structural Transitions for V(acac)3- and Ru(acac)3-based Flow Battery Electrolytes Using X-Ray Absorption Spectroscopy** (ThB4c)

Jonathan Kucharyson, Jason Gaudet, Brian Wyvratt, Levi Thompson (University of Michigan)

The charge storage mechanisms and structural changes for vanadium(III) acetylacetonate and ruthenium(III) acetylacetonate non-aqueous electrolytes for flow battery applications were characterized using bulk electrolysis (BE) and X-ray absorption spectroscopy, and further compared to DFT structure optimization calculations using Gaussian 09. The XANES spectra was used to quantify that 80±20% and 120±20% of the charge is stored on the ruthenium atom for the positive and negative reactions respectively for ruthenium(III) acetylacetonate, and no charge is stored on the vanadium atom for the positive and negative reactions of vanadium(III) acetylacetonate. EXAFS analysis reveals minimal structural changes for the negative reaction of ruthenium(III) acetylacetonate which is verified through reversible charge/discharge and DFT Ru-O bond length calculations, while the positive reaction EXAFS shows evidence of ligand distortions resulting in irreversible changes in the electrochemistry. DFT and additional BE experiments provide evidence of increased V-O bond length changes for the negative reaction of vanadium(III) acetylacetoante resulting in ligand shedding, and the formation of vanadyl acetylacetonate during the positive reaction which then reacts with the acetonitrile solvent at low potentials.

3:00 PM **Rational Design of Low Cost Electrode Catalysts for Fuel Cell Applications** (ThB4d)

Heather M. Barkholtz (Northern Illinois University), *Lina Chong, Zachary B. Kaiser, Di-Jia Liu* (Argonne National Laboratory)

Proton exchange membrane fuel cells (PEMFCs) are a promising technology for transportation applications due to their high power densities, the ability to respond rapidly to load variability, and low operating temperatures. Before widespread commercialization can be realized, two major hurdles must first be overcome. The cathodic oxygen reduction reaction (ORR) is sluggish, and improvements in catalyst kinetics must be achieved. In addition to scientific advancements in cathodic ORR activity, there must also be a reduction or elimination in the use of costly platinum group metal (PGM) catalyst materials [1].

At Argonne National Laboratory, we have developed new "support-free" non-PGM materials to replace platinum cathode electrocatalysts for PEMFCs[2,3]. Our approach uses transition metal and nitrogen – doped carbon materials prepared from high surface area metal-organic framework precursors as electrocatalysts for the oxygen reduction reaction (ORR). For example, we have reported a one-pot all solid-state synthesis technique to prepare iron-doped MOFs which once pyrolyzed afford highly ORR active catalysts, approaching performance targets set by U.S. DOE for automotive applications[4,5]

In this work, we report recent developments in rationally prepared non-PGM electrocatalyst materials for PEMFC applications. Both the design and synthesis of MOF-based precursors as well as thermal activation and processing conditions are optimized for ORR activity at the fuel cell level. Electrocatalytic activities and physical properties of the catalysts are reported with an emphasis on understanding active site formation.

[1]. Morozan, A.; Jaouen, F. Energy Environ. Sci. 2012, 5, 9269.

[2]. Shengqian MA, Gabriel Goenaga, Ann Call, and Di-Jia Liu, Chemistry: A European Journal 2011, 17, 2063.

[3]. Dan Zhao, Jiang-Lan Shui, Chen Chen, Xinqi Chen, Briana M. Reprogle, Dapeng Wang, and Di-Jia Liu, Chem. Sci. 2012, 3, 3200.

[4]. Dan Zhao, Jiang-Lan Shui, Lauren R. Grabstanowicz, Chen Chen, Sean M. Commet, Tao Xu, Jun Lu, and Di-Jia Liu, Advanced Materials 2014, 26, 7.

[5]. Barkholtz, H. M.; Chong, L.; Kaiser, Z. B.; Xu, T.; Liu, D. J. Catalysts 2015, 5, 955.

3:20 PM **Environmental Transmission Electron Microscopy Study of Composition Redistribution for Pt-Ni Octahedral Electrocatalysts for Reduction of Oxygen** (ThB4e)

Yung-Tin Pan, Jianbo Wu, Hong Yang (University of Illinois at Urbana-Champaign)

Dynamic elemental distribution of carbon-supported Pt-Ni octahedral (Oh) nanocrystal was studied using environmental transmission electron microscope (ETEM) under thermal annealing conditions. The as-made Pt-Ni Oh nanocrystal was inhomogeneous in atomic distribution with a Pt rich shell and core region with a Ni rich region sandwiched in between which provided the driving force for atomic diffusion and redistribution. Upon mild annealing in vacuum at enhanced temperatures the migration of paired dislocations, which was the tracer of the boundary between the Pt rich surface and Ni rich sub layer, was observed to move towards the surface over time indicating Pt/Ni counter diffusion taking place. The migration of dislocations was found to follow first order decay as a function of time, suggesting a Fick's law like behavior where the diffusion coefficient was approximated. XPS study on as-made and post annealed (under vacuum) Oh Pt-Ni nanocrystals agreed with the observation in the in-situ ETEM where the Ni surface ratio increased significantly after thermal treatment. The thermally treated Pt-Ni Oh nanocrystal showed significant improvement in catalyzing oxygen reduction reaction (ORR) as compare to the as-made nanoparticles. Our result indicates that optimization of Pt and Ni atom distribution can be achieved through thermal treatment and mild under vacuum in a controllable and quantitative fashion while preserving the desired {111} surface dominant octahedral shape.

<u>Multiphase CFD Tutorial</u>

Thursday, March 3, 2016 (Crown Room, **ThB5**)

Chair: *Reza Mostofi* (UOP/Honeywell)

<u>Tutorial Description</u>: Commercial CFD codes are widely used for design and performance improvement of various fluidized bed reactors, such as the FCC reactors in the oil industry, new fluidized bed reactors for polysilcon production for solar cells and future biomass reactors. Transport in blood vessels is also modeled using multiphase CFD.

The objective of this tutorial is to review the basic multiphase flow conservation laws and to show how to use CFD codes to obtain useful design information. The example to be used is the formation of bubbles in a gasifier and their possible elimination, as described in "Computational Techniques", Nova Science Publishers (2009).

4:00 PM **Multiphase Conservation Laws and Their Constitutive Equations** (ThB5a)

Dimitri Gidaspow (Illinois Institute of Technology)

Conservation laws of mass, chemical species, momentum and energy for each phase, gas, liquid and solid, will be derived using the Lagrangian approach, as is done in transport phenomena courses for one phase. The only new variable in multiphase flow is the volume fraction of phase i. The constitutive equations are obtained from kinetic theory of granular flow.

4:55 PM **Demonstration of IIT Multiphase CFD Code for Reactor Improvement** (ThB5b)

Dimitri Gidaspow (Illinois Institute of Technology)

Our CFD code will be run for the Westinghouse 3 meter fluidized bed, pages 428-431 in "Computational Techniques" by Gidaspow and Jiradilok, Nova Science, 2009. The code runs for 5 minutes for a 10 second run. Bubbles are produced, as observed at Westinghouse. Such bubbles can be eliminated by use of large particles. It will be shown how to obtain sufficient turbulence to get good fluidization and good heat transfer.

The Hydrogen Economy

Thursday, March 3, 2016 (Ballroom, **ThC1**)
Chair: *David Shonnard* (Michigan Technological University)
Co-chair: *Jui-Kun Peng* (Argonne National Laboratory)

4:00 PM **A Fifty+ Year Perspective on Sustainability** (ThC1a)
Robert Anderson (Illinois Institute of Technology)

Dedicated to the memory of Henry Linden, pioneer in establishing policy for dealing with the energy, environment, and economic aspects of sustainability

One of the giants of chemical engineering, Professor John McKetta, gave a lecture at the Chicago Section of AIChE in 1962, stating his opinion that the time was not far off when every company in the manufacturing business would be able to quantify the waste material leaving their property in the air, water, and solid waste. John was AIChE President at the time. Few in the audience could imagine such a fantasy becoming reality. At the same time the automobile industry was being asked to design engines that reduced emission of unburned hydrocarbons and carbon monoxide. When they tested the only catalyst effective for this task, platinum on alumina, they found that the catalyst died in only a few days, poisoned by the lead, which had been added in the form of tetraethyl lead to the gasoline to improve its antiknock properties. The auto companies stood their ground. "No catalytic converters until lead-free gasoline widely available." The oil companies were just as fixed in their position. "No lead-free gasoline until your cars have catalytic converters." Eventually the Environmental Protection Agency stepped in and ended the standoff.

In the 1970's, Professor Henry R. Linden of IIT and the Institute of Gas Technology began a dedicated journey to address the complex issue of sustainability of the world. His first contribution was to craft a clear definition of sustainability and a pathway to achieving it.

- "A sustainable global energy system must be able to provide all of the useful energy services required for continued improvements in human social and economic well-being and physical mobility without depleting significant resources and relying on exhaustible primary energy sources or causing dissipative materials flows into the biosphere that threaten to destabilize it."
- "Likely endpoint is electrification of most stationary energy services and use of non-fossil hydrogen as the dominant transportation fuel and energy storage medium for electricity from intermittent sources."

This paper captures the insights gained over more than three decades of educating IIT students in these important principles in a class now called E3, for energy, environment and economics. It is clear that Professor Linden's perspective is applicable to transportation, water supply and conservation, production and distribution of food, design of buildings and cities, use of labor-saving devices, public health, eradication of poverty, and stewardship of natural resources.

E3 began with the symbol of the three-legged stool, indicating graphically that forgetting one leg of the stool will lead to an embarrassing crash. When considering a new energy source, be sure to consider the environmental impact and the economics, both first cost and operating cost. Be sensitized to the reality that any solution to environmental damage carries with it energy and economic components. And, any economic enterprise must be scrutinized for its energy consumption and environmental impact. As societal problems have grown, we have had to add politics, sociology, education, culture, and ethics to the simple three E's.

Students have extended the E3 discipline to address infant mortality caused by contaminated water, the energy and water implications of agricultural irrigation, true costs of food production and distribution, the impact of political corruption on human welfare, provision of electric power to remote regions of developing countries, the disruption caused by rising ocean levels, the importance of education of the populace and their political leaders, new energy storage technologies, architectural impacts on energy and the environment, city planning, public transportation, new transportation technologies, public health implications of coal combustion, after effects of deforestation, use of geothermal energy, harnessing the energy of waves and tides, thermal pollution of rivers, urban farming, extinction of biological species, and the effect of personal choices on their carbon footprint.

E3 is a graduate level chemical engineering course. As students from mechanical engineering, environmental engineering, civil engineering, architecture and architectural engineering, and food safety have enrolled, the students teach and learn from each other, recognizing that complex problems will not be solved within the narrow reach of a single academic discipline.

4:20 PM **Experimental Investigation of a Hybrid Photoelectrochemical Hydrogen Production System** (ThC1b)
Canan Acar, Ibrahim Dincer (University of Ontario Institute of Technology)

This study aims to experimentally investigate a hybrid chloralkali-photoelectrochemical system for hydrogen production by splitting water and converting the by–products into useful industrial products, namely chlorine and sodium hydroxide. This hybrid system maximizes the utilized solar spectrum by combining photochemical and electrochemical processes. Furthermore, by using electrodes instead of electron donors for photochemical hydrogen production, the hybrid system minimizes chemical waste generation and health hazards associated with the utilization of these chemicals. The system is tested at 4 different temperatures (20, 40, 60, and 80°C) and 3 different light settings (no light, 600 W/m^2, and 1200 W/m^2). The results show that the reactor responds light by generating photocurrent. The hydrogen production rate increases with increasing temperature and light intensity.

Under no light conditions at 20°C, the present system produces about 145 mL/h hydrogen while it generates 295 mL/h hydrogen at 80°C under 1200 W/m^2 irradiation.

4:40 PM **NaBH4 "Wrapped in Graphene": Significantly Improved the Hydrogen Storage Capacity and Reversibility through Nanoencapsulation** (ThC1c)
Lina Chong (Argonne National Laboratory), *Jianxin Zoub, Xiaogin Zengb, Wnjiang Dingb, Di-Jia Liua* (Shanghai Jian Tong University)

Hydrogen powered vehicles are anticipated to play a key role in the next-generation, zero-emission transportation technology. These vehicles require an onboard hydrogen system that can store and deliver large amount of H2 at moderate temperatures and fast rate [1]. Alkaline boron hydride, due to its high theoretical capacity (e.g. NaBH4 > 10 wt. %), has been regarded as a promising H2 adsorbent for the transportation. The past studies found, however, that alkaline boron hydrides suffer poor regenerability and high level of byproduct contamination during solid-state dehydrogen-rehydrogenation reactions. For example, upon extraction of H2 from hydride, the decomposed components such as boron and alkaline metal will escape to gas phase or migrate away on the support surface, rendering them difficult to be recaptured and regenerated during the charging cycle.

In this work, we reported a new approach using a simple, robust wet chemistry method to prepare hydrogen storage composite by encapsulating nano-dimensional NaBH4 inside of a light-weight, single layer "graphene wrapper" [2]. Such composite structure restricts the hydride phase segregation/agglomeration, maximizes graphene-catalyzed hydride de/re-hydrogenation capacities, significantly improves the H2 charge/recharge kinetics, and prevents the escape of dehydrogenation products. As the results, a steady and high reversible H2 storage capacity of 7.0 wt.% was achieved with fast H2 uptake. Furthermore, no byproduct was detected in the produced hydrogen. In this presentation, I will discuss the way to design and synthesis of graphene-capsulated hydride composite, its chemical and physical characterization, as well as hydrogen storage measurements, such as, DSC, PCT, etc.

[1]. L. Schlapbach, A. Zuttel, Nature 2001, 414, 353.
[2]. L. N. Chong, X. Q. Zeng, W. J. Ding, D. J. Liu, J. X. Zou, Adv. Mater. 2015, 27, 5070.

5:00 PM **Mechanical Property Study of Metal-Organic Framework** (ThC1d)
Zhi Su, Kenneth Suslick (University of Illinois at Urbana-Champaign)

Metal-organic frameworks could have extremely high surface areas with tunable porosities and variable chemical and physical properties. The issues of chemical, thermal and mechanical stabilities are critical to their effect use for a variety of applications, particularly in understanding what requirements are necessary to provide structural integrity and porosity after removal of solvates. We have successfully synthesized narrow size distributed zeolitic imidazolate framework-8 (ZIF-8) crystals (550 nm - 2.3 um), which was constructed by 2-methylimidazolate with Zn(II). We have investigated morphological deformation of individual ZIF-8 crystal under compression and revealed the function of volume change with applied pressure. The most striking feature is that the existence of solvates in the pores has strengthen the rigidity of ZIF-8, which shattered at a very low applied force. Our results have offered a new insight of relationship between structure, morphology, and mechanical property, which would provide new direction for future crystal engineering work.

5:20 PM **Low-Temperature Preferential Oxidation of Carbon Monoxide on Pt3Ni Alloy Nanoparticle Catalyst with Engineered Surface** (ThC1e)
Zhenmeng Peng, Sang Youp Hwang, Eric Yurchekfrodl, Changlin Zhang (University of Akron)

Preferential oxidation of carbon monoxide (PROX) in a large excess of hydrogen has received considerable interest for applications requiring the use of clean H2, including proton exchange membrane fuel cell (PEMFC) technology and ammonia synthesis. It is because that the typical H2 production processes by reforming hydrocarbons and diesel fuels generate CO as a byproduct, which is notorious poisoning species and readily deactivating many catalysts. There is thus a need for selective removal of CO before H2 can be used for these applications.

We report the use of Pt-Ni alloy nanoparticles with well-engineered surfaces as highly active and selective PROX catalyst. Specifically, the researched octahedral Pt3Ni alloy nanoparticle catalysts, which are exclusively enclosed by the (111) surface, exhibit both high PROX activity and 100% selectivity from RT all the way till around 100 °C. The much promoted CO oxidation kinetics on octahedral Pt3Ni was attributed to significantly decreased Ea comparing to spherical Pt3Ni and Pt (~40.0 kJ/mol vs. 56.9 and 66.3 kJ/mol) and the presence of both Pt and Ni active sites on the engineered (111) surface, which can work synergistically to activate and react CO and O2. The 100% PROX selectivity was associated with the unique (111) surface geometry of the octahedral Pt3Ni and the big difference in the adsorption energy of CO and H2 on the surface, which help with suppressing H2 from adsorption and oxidation.

Drug Delivery II

Thursday, March 3, 2016 (Armour Dining, **ThC2**)
Chair: *Georgia Papavasiliou* (Illinois Institute of Technology)
Co-chair: *Brittany Hartwell* (University of Kansas)

4:00 PM **Agrochemical likeliness: Why Agrochemicals Differ from Drugs?** (ThC2a)
Saurabh Shukla (University of Illinois at Urbana-Champaign)

Agrochemical discovery process can be expedited by the knowledge of important physiochemical properties of the molecule. Agrochemicals are generally sprayed exogenously and face harsher environments than orally administered drugs. Also, transport of an agrochemical into the plant cell does not resemble the delivery of drugs in humans. Lipinski's rules outline five chemical features that define likeliness. We investigate important chemical features that define agrochemical likeliness by computationally analyzing the properties of approved agrochemicals. We also comment on how agrochemicals differ from an orally administered drug. Such a knowledge can reduce enormous effort gone into screening of large libraries of compounds and to synthesize new agrochemicals.

4:20 PM **Antibiotic Probiotics Reduce Salmonella in GI Tract of Animals** (ThC2b)

Yiannis Kaznessis, Brittany Forkus, Kathryn Geldart
(University of Minnesota)

Foodborne gastrointestinal infections are significant causes of morbidity and mortality worldwide. Alarmingly, often because of the extensive, non-therapeutic use of antibiotics in agriculture, foodborne bacteria are emerging that are resistant to our most potent drugs.

We will discuss a novel approach to reduce the use of antibiotics in food-producing animals and to treat gastrointestinal infections. We engineer probiotic, lactic acid bacteria (LAB) that express and release antimicrobial peptides (AMPs). LAB are part of the gastrointestinal microflora and can be safely delivered with known benefits to humans and animals. AMPs are proteins that can be readily produced by LAB. One unique aspect of our approach is the use of synthetic promoters that precisely regulate the delivery of AMP molecules.

At the heart of proposed efforts are multiscale models that guide explanations and predictions of the antagonistic activity of recombinant LAB against pathogenic strains. Models are developed to quantify how AMPs kill bacteria at distinct but tied scales. Using atomistic simulations the various interaction steps between peptides and cell membranes are explored. Mesoscopic models are developed to study ion transport and depolarization of membranes treated with AMPs. [1] Stochastic kinetic models are developed to quantify the strength of synthetic promoters and AMPs expression [2].

Experimentally, we engineer lactic acid bacteria to inducibly produce antimicrobial peptides. We have developed a library of synthetic biological constructs. [3] We test modified bacteria against pathogenic bacteria. We will present in vitro results against salmonella and enterococcus [4-6]. We will also present proof-of-concept results of in vivo studies with turkey poults and mice.

[1]. Kaznessis Y, “Multiscale Models of Antibiotic Probiotics”, Curr Opin Chem Eng, 2014, 1;6:18-24

[2]. Smadbeck P, Kaznessis YN. “A closure scheme for chemical master equations. Proc Natl Acad Sci U S A”. 2013 Aug 27;110(35):14261-5. doi: 10.1073/pnas.1306481110.

[3]. Volzing K, Billiouris K, Kaznessis YN. “proTeOn and proTeOff, New Protein Devices That Inducibly Activate Bacterial Gene Expression”, ACS Chem Biol. 2011, 6:1107-1116.

[4]. Volzing K, Borrero J, Sadowsky MJ, Kaznessis YN. “Antimicrobial Peptides Targeting Gram-negative Pathogens, Produced and Delivered by Lactic Acid Bacteria.” ACS Synth Biol. 2013. 15;2(11):643-50. doi: 10.1021/sb4000367 .

[5]. Borrero J, Dunny G, Kaznessis YN, " Modified Lactic Acid Bacteria Detect and Inhibit Multiresistant Enterococci." ACS Synth Biol. 2014, 10.1021/sb500090b

[6]. Geldart K, Borrero J, Kaznessis YN. “A Chloride-Inducible Expression Vector for Delivery of Antimicrobial Peptides Against Antibiotic-Resistant Enterococcus faecium”, Applied and Environmental Microbiology, 2015 Jun 1;81(11):3889-97. doi: 10.1128/AEM.00227-15.

4:40 PM **Engineering Albumin-hitchhiking Vaccines for Type 1 Diabetes** (ThC2c)

Haipeng Liu, Meng Li, Jingchao Xi (Wayne State University)

Vaccine approaches to restore antigen-specific immune tolerance to pancreatic beta-cell antigens without global immune suppression are potential therapeutic interventions for Type 1 diabetes (T1D). However, a method for realizing both efficacy and safety is yet to be developed. A major challenge in the development of effective vaccines is efficient delivery of vaccine components to antigen presenting cells (APCs) in lymphoid organs, where the orchestrations of immune cells are initiated.

We recently demonstrated that both the efficacy and safety of subunit vaccines can be dramatically enhanced by rational molecular design which target lymphoid organs via ‘albumin-hitchhiking’, a mechanism by which structurally optimized molecular vaccines are engineered with a lipophilic albumin-binding tail and follow subcutaneous injection, exhibit dramatic increases in LN accumulation via in situ complexation and transport with endogenous albumin, leading to 30-fold augmentation in CD8+ T-cell priming while greatly reducing systemic toxicity (Liu et al. Nature, 2014). Here we translate these findings to deliver molecular vaccines to LNs, where they can be efficiently filtered by resident phagocytes and accumulate, promoting antigen-specific tolerance. Treatment of NOD mice with albumin-hitchhiking vaccines significantly delayed and reduced the incidence of diabetes. This is associated with significant suppression of antoreactive CD4 T cells and increased frequency of regulatory T cells, as well as increased suppressive cytokine productions.

5:00 PM **Drug Selectivity Mechanism of Kinases** (ThC2d)

Zahra Shamsi, Diwakar Shukla (University of Illinois at Urbana-Champaign)

Abstract: One of the key challenges facing the pharmaceutical industry is the design of potent and selective small molecule (drug) modulators of biological activity. Drug selectivity plays a crucial role in designing molecules with limited side effects. Here, we investigate the selectivity mechanism of a successful drug for cancer treatment, Gleevec [1-3]. The evolutionary pathway between the modern kinases, c-Src and Abl has been recreated through molecular dynamics simulations of their common ancestors to find an atomistic mechanism responsible for the differences in their drug binding behavior. Our preliminary results show that the conformational differences between the ancestral kinases could be responsible for the Gleevec selectivity differences between c-Src and Abl.

[1]. Y.-L. Lin, Y. Meng, W. Jiang, and B. Roux, “Explaining why Gleevec is a specific and potent inhibitor of Abl kinase.,” Proc. Natl. Acad. Sci. U. S. A., vol. 110, no. 5, pp. 1664–9, 2013.

[2]. D. Shukla, Y. Meng, B. Roux, and V. S. Pande, “Activation pathway of Src kinase reveals intermediate states as targets for drug design.,” Nat. Commun., vol. 5, p. 3397, 2014.

[3]. C. Wilson, R. V Agafonov, M. Hoemberger, S. Kutter, A. Zorba, J. Halpin, V. Buosi, R. Otten, D. Waterman, D. L. Theobald, and D. Kern, “Using Ancient Protein Kinases to Unravel a Modern Cancer Drug’s Mechanism,” Nature, vol. 5287, no. 1995, pp. 201–206, 2014.

5:20 PM **The Role of Natural Fluids in Studies of In-Vitro Pulmonary Drug Delivery** (ThC2e)

Benjamin King, Jennifer Fiegel (University of Iowa)

Upon delivery to the body and interaction with bodily fluids, drug carriers are instantaneously coated with proteins and other biomolecules, forming a protein corona on the particle surface. It is this protein-coated surface that the body “sees” and that determines the subsequent fate of the particles within the body. In our work, polystyrene particles were exposed to either bronchoalveolar lavage fluid or serum and were subsequently well characterized prior to exposure to lung cells. The effect of exposure to each of these fluids was studied to investigate the significance of fluid environment on model drug carrier behavior. Exposure to blood or lung fluid results in different particle behaviors indicating that particle behavior in one biological system or organ is not necessarily translatable to other systems. While lung fluids and serum have similar proteomics, they interact with particles in markedly different ways. Therefore, a particle system may have unique cellular and tissue responses depending on route of exposure. This is an important consideration for in vitro studies of pulmonary drug delivery. Serum contains many essential nutrients that assist in cell growth both in vivo and in vitro, but its presence during drug exposures can result in behavior that is not true to the pulmonary environment. Thus, as in vitro models of pulmonary drug delivery improve, naturally sourced lung fluids should be incorporated to improve model system prediction of in vivo behavior.

<u>Process Safety III</u>

Thursday, March 3, 2016 (Alumni Lounge, **ThC3**)
Chair: *Robert J. Weber* (PSRG)
Co-chair: Brenton L. Cox (Exponent Inc.)

4:00 PM **Quantitative Risk Assessment Technological Advancements** (ThC3a)

Jesse Calderon (Baker Risk Engineering and Risk Consultants, Inc.)

Facility Siting Studies (FSS) and Quantitative Risk Assessments (QRA) estimate the potentially hazardous consequences and cumulative process risk posed by operation of a facility, respectively. FSS and QRAs are widely used in the chemical industry, with the scope of these studies potentially including onsite and/or offsite risk to personnel; although less common, the results of a QRA can also be expressed in purely economic or environmental terms.

As QRAs have become more commonplace in the chemical industry, a number of advancements in the way these calculations are performed have allowed for a reduction in the conservatism built into the mathematical models and an increase in the accuracy of the risk results. Several major advancements include, but are not limited to: a better understanding of occupant vulnerability associated with exposure to facility hazards, leak tightness testing for toxic mitigation of shelter-in-place buildings, probability of ignition calculations, API RP 756 for the siting of portable tents, and field testing capabilities for procurement of new data to be used in consequence and risk assessments. This presentation will review a brief introduction into consequence modeling and QRAs, the recent advancements and potential future advancements in QRAs, and how these advancements relate to Recognized and Generally Accepted Good Engineering Practice (RAGAGEP).

4:20 PM **Using Bow Ties for Process Hazards Analysis** (ThC3b)

Ngoc (Annie) Nguyen (PSRG)

This presentation presents Bow Tie methodology and how and when this tool may be used for assessing and presenting Process Hazards Analysis and comparison to other PHA methods.

4:40 PM **Combining Traditional UOP HAZOP Analysis with Dynamic Simulation a New Process Safety / Risk Assessment Tool** (ThC3c)

Scott M. Wozniak (UOP)

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

This paper shows how our current UOP HAZOP methodology is supported by dynamic simulation and modeling techniques. By leveraging this process technology, UOP can now deliver more robust HAZOP studies by integrating our current UOP Process Technology library of UNISIM flowsheet templates in all phases of the HAZOP work process.

We will show how dynamic simulation can determine consequences of deviations from normal design exactly and how this tool can potentially identify new unknown hazards and safety issues.

5:00 PM **A Comparison of Water Distribution Resilience Metrics** (ThC3d)
Michael Bynum, Carl Laird (Purdue University), Terra Haxton, Regan Murray (Environmental Protection Agency), Katherine Klise (Sandia National Laboratories)
Resilience of water distribution systems is vital for the health and lives of people all around the world. However, measuring resilience is not trivial. Many resilience metrics have been developed, including topological, hydraulic, water quality, and entropy metrics, among others. These metrics measure different aspects of resilience; some metrics might be harder to interpret than others. This is especially true for resilience metrics that do not directly utilize the performance metric of interest. For example, topological metrics only use the network layout which has no direct information on impact to the customer such as the amount or quality of water delivered. Additionally, different metrics require differing amounts of information and have differing computational costs. For example, some metrics require the results of hydraulic simulations while others only need the network layout.
In this work, we review and compare water distribution system resilience metrics. Each metric is evaluated across multiple networks in order to determine how well the metrics agree with each other. Multiple scenarios, including both power outages and pipe leaks, are used to identify the robustness of each metric. The entire analysis is performed in Python with WNTR, a Water Network Tool for Resilience. WNTR explicitly models leaks and pressure-dependent demands in order to accurately capture water distribution system performance.

5:20 PM **Chemical Facility Anti-Terrorism Standards, 6 CFR part 27** (ThC3e)
Gregory Wolff (U.S. Homeland Security)
CFATs 101 presentation, and Q&A session about compliance with CFATS.

Process Design and Optimization II

Thursday, March 3, 2016 (Herman Lounge, **ThC4**)
Chair: *Urmila Diwekar* (Vishwamira Research Institute)
Co-chair: *Rajesh Gattupalli* (UOP/Honeywell)

4:00 PM **Design and Characterization of a Millifluidic Herringbone Mixer** (ThC4a)
Joseph Whittenberg, Vivek Kumar, Keegan Lane, Sumit Verma, Heeral, Paul J. A. Kenis (University of Illinois at Urbana-Champaign)
Mixing in systems at the microscale and macroscale has been well characterized, but less is known about mixing at the millifluidic scale (at least 1 dimension close to 1 mm in size). Millifluidic mixing systems are particularly valuable because they can be used in lab scale production (grams per day) of organic compounds and nanoparticles. Additionally, similar microfluidic platforms require specialized fabrication facilities and are typically not amenable to mass production.
In this work we scaled-up the highly utilized microfluidic herringbone mixer design to mix solutions in a high throughput manner. Mixer dimensions were optimized using COMSOL, then fabricated by milling polymethylmethacrylate (PMMA) and bonding the milled PMMA to a flat PMMA substrate. Dyes were used to quantify the extent of mixing (roughly 89 – 96%) at various flow rates (0.2 – 13 mL/min) and positions on the device. Monodisperse gold nanoparticles were synthesized using the device to demonstrate one potential application for the scaled-up mixer.

4:20 PM **A Parallel Dynamic Optimization Approach for Inverse Problems in Water Distribution Systems** (ThC4b)
Jose Rodriguez, Carl D. Laird (Purdue University)
Reliable modeling of dynamic systems frequently requires accurate knowledge of inputs and parameters to be computed from system measurements. In this talk, we present a parallel approach for dynamic optimization applied to inverse problems in water distribution systems. Previous work presented an interior-point approach that made use of a Schur-complement decomposition in the linear solution of the KKT system to solve dynamic optimization problems in parallel. This approach was particularly advantageous for problems with few states but many algebraic variables. Water distribution networks typically include thousands of junctions and pipes, but relatively few storage tanks, resulting in dynamic systems with precisely these properties. To develop reliable models for improving system operation, there is a need for reliable estimation of water consumption from flow and pressure data. To allow accurate estimation of the hydraulic parameters in real time, we have developed an optimization formulation. Given the spatial sparsity of data, we include a regularization term in the objective function that accounts for spatial correlation of the demand values. In addition, to mitigate the effect of gross measurement errors, we studied different robust estimators that could yield less biased estimates. For large networks, the optimization problem can become prohibitively large for real-time computation, and we demonstrate the parallel speedup that is possible using the Schur-Complement decomposition approach.

4:40 PM **Heterogeneous Multi-Agent Optimization Framework to Solve Large Scale Process System Engineering Problems** (ThC4c)
Berhane H. Gebreslassie, Urmila M. Diwekar (Vishwamitra Research Institute)
Multi-agent optimization is a nature-inspired optimization method, which supports cooperative search by group of algorithmic agents connected through an environment with certain predefined information sharing protocol. The multi-agent optimization framework provides a platform for combining various algorithms from different background and exploits the strength that each algorithm possesses. Large scale

process system engineering problems are non-convex and combinatorial in nature and they involve multiple local optimal and few combinatorial solutions. Therefore, MAOP approach is an ideal candidate solution method for process system engineering problems because it avoids getting stuck in local optima with a better computational performance. An agent in the MAOP framework is formed by combining an algorithmic procedure, a communication protocol between the algorithmic procedure and the global information sharing environment, the algorithmic procedure specific initialization and output retrieving methods. In this context, an agent can be defined as a distinct, autonomous software entity that is capable of observing and altering its environment. An agent evaluates a given task that contributes directly or indirectly to the advancement of it's surrounding Siirola et al (2003). The agents are combined into a cohesive system where the individual agents interact through the global information sharing environment. The MAOP framework exhibits both the aggregate properties of the individual agents, and superior properties resulting from the interactions among the individual agents. In this nature inspired MAOP platform, the overall behavior is not governed by a strong, centralized control rather by the individual algorithms that make up the framework operate autonomously. Hence, the MAOP framework has the capability to solve problems from different background with better computational efficiency. The MAOP framework could be homogenous MAOP developed based on same multiple algorithmic agents or heterogeneous MAOP (HTMAOP) developed based on diverse algorithmic agents.

The platform is validated using a benchmark problems and a computer-aided molecular design (CAMD) problem. A solvent selection CAMD problem is formulated as a mixed integer nonlinear programming (MINLP) in which solute distribution coefficient of a candidate solvent is maximized subject to structural feasibility, thermodynamic property and process constraints. The model simultaneously determines the optimal decisions that include the size and the functional groups of the candidate solvents. In developing the HTMAO framework, efficient ant colony optimization (EACO) algorithm, efficient genetic algorithm (EGA) and efficient simulated annealing (ESA) are considered as distinct algorithmic agents. We illustrate this approach through a real world case study of the optimal design of solvent for extraction of acetic acid from waste process stream using liquid-liquid extraction. The UNIFAC model based on the infinite dilution activity coefficient is used to estimate the mixture properties. The results show that quality of the objective function and the computational efficiencies are improved by a factor ranged from 1.475 to 4.137. The new solvents proposed in this work are with much better targeted thermodynamic properties compared to the solvents proposed so far in previous studies.

[1]. Siirola JD, Hauan S, Westerberg AW. Toward agent-based process systems engineering: proposed framework and application to non-convex optimization. Computers and Chemical Engineering 2003; 27, 1801-181.

[2]. Gebreslassie BH, Diwekar UM. Homogenous multi-agent optimization for computer aided molecular design: case study solvent selection problem. Computers and Chemical Engineering.

[3]. Diwekar U, Xu W. Improved genetic algorithms for deterministic optimization and optimization under uncertainty. Part I. algorithms development. Industrial and Engineering Chemistry Research 2005; 44, 7132–7.

[4]. Kim K, Diwekar UM. Efficient combinatorial optimization under uncertainty. 1. Algorithmic development. Industrial and Engineering Chemistry Research 2002a; 41, 1276–84.

5:00 PM **Numerical Optimization of Gasoline Storage Tank Ventilation** (ThC4d)

Chenn Zhou, Bin Wi (Purdue University Calumet)

Above ground gasoline storage tanks always experience problems in the winter. Snow is blown into the tanks through their center and peripheral vents and accumulate on their internal floating roofs. The size of the ventilation opening must be large enough to allow outside air to flow in and dilute gasoline vapor inside the tank, but should not be too large such that snow could be blown in. An alternative design for peripheral vents that can eliminate the problem is desired. Computational Fluid Dynamics (CFD) is employed to model the flow around and inside the storage tank. In addition to modeling the current tank, two modified storage tanks are modeled and proposed as possible solutions to the problem. To ensure the proposed modified tanks meet the industry standards, a tank design based on the industry standards is modeled and is used as a benchmark. An optimized design for current stage has been achieved through comparing the differences in the velocity field and air mixture of the tank among different configurations.

5:20 PM **A Novel Approach to Improve the Barrier Properties of Polyethylene Terephthalate** (ThC4e)

Kazem Majdzadeh Ardakani, Saleh A. Jabarin (University of Toledo)

This study is to investigate the contribution of the active and passive oxygen barrier approaches by modifying nanoparticles with unsaturated fatty acids to act as an oxygen scavenger. This approach can improve the dispersion of layered silicates into the PET as well as the barrier properties. Montmorillonite (MMT) and Cloisite 30B nanoclays were modified by long-chain oleic acid and identified as ol-MMT and ol-30B, respectively. The dispersion and compatibility of prepared PET/modified clay nanocomposites were examined by XRD, DSC, TGA, and TEM. Mechanical and barrier properties of samples were also examined. Fourier transform infrared spectroscopy and X-ray diffraction (XRD) results revealed that the fatty acid was associated with the clay surface and that the gallery spacing of the layered silicates was expanded. In the case of ol-MMT, a disordered structure of layered silicates was achieved. PET/clay nanocomposites were prepared with modified ol-MMT and modified ol-30B by using a twin screw extruder. Significant improvements in morphology, mechanical and barrier properties of stretched PET/clay nanocomposites were achieved.

Job Search Strategies
Thursday, March 3, 2016 (Armour Conference Room, **ThC5**)
Chair: *BJ Engelhardt* (Illinois Institute of Technology)

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

4:00 PM **Finding Your Market** (ThC5a)
Akshar Patel (Illinois Institute of Technology)

4:55 PM **Making Your Connections** (ThC5b)
Akshar Patel (Illinois Institute of Technology)

Process Modeling and Estimation
Friday, March 4, 2016 (Ballroom, **FrA1**)
Chair: *Victor Zavala* (University of Wisconsin)
Co-Chair: *Jeffrey M. Zalc* (BP)

9:45 AM **A Meal Detection and Carbohydrate Estimation Algorithm Based on CGM Data for Use in AP Systems** (FrA1a)
Sadiqeh Samadi, Kamuran Turksoy, Jianyuan Feng, Iman Hajzadeh, Mert Sevil, Ali Cinar (Illinois Institute of Technology)
Diabetes is a chronic metabolic disease in which patients suffer from hyperglycemia (high blood Glucose concentration) either because insulin production is impaired, or the body's cells do not respond properly to insulin [1]. Artificial pancreas (AP) control systems offer an important improvement in regulating blood glucose concentration with type 1 diabetes [1]. Automatic handling of the deviation of blood glucose concentration (BGC) from control target range as a result of meal effects is one of the biggest challenges of AP systems, particularly when the controller is not informed about the meal time and its carbohydrate amount by manual announcement. An AP control system equipped with meal detection and carbohydrate estimation module has the potential to make more appropriate insulin decisions and have better performance in blood glucose regulation.
Method: In this study, a trend analysis based algorithm is proposed to estimate the time and amount of carbohydrate intake at meals (snacks) based on continuous glucose monitoring (CGM) data and subcutaneous insulin delivery data from insulin pump. Frequent data of subcutaneous glucose concentration from a CGM are used to describe meal effects on glucose variation. The algorithm has three steps. The noise of measured glucose is filtered in the first step. In the second step, the effect of meal on BGC variation is modeled by some qualitative variables. Using qualitative trend analysis (QTA) technique, BGC time series is described by a set of qualitative variables. Each qualitative variable has a different combination of first and second derivative signs. Meals are detected based on the sequence and patterns of these qualitative variables. In the third step, a fuzzy system estimates the carbohydrate content of the meal using measured glucose and subcutaneous infused insulin.
Results: The algorithm is tested on data of five different T1D patients participating in clinical experiments. Sensitivity, defined as the ratio of number of correctly identified meals and snacks to the total number of meals and snacks, is 0.92. False positive ratio defined as the ratio of false detections to total detections is 0.11. The average increase in BGC between the beginning of a meal and the time of detection varies from -30 to 10 mg/dl for different patients. The average magnitude of error in carbohydrate meal size estimation is 16.5 g.

10:05 AM **Real-Time Estimation of Plasma Insulin Concentration Using Glucose Measurements in Patients with Type 1 Diabetes (FrA1b)**
Iman Hajizadeh,Kamuran Turksoy, Sadiqeh Samadi, Jianyuan Feng, Mert Sevil, Ali Cinar (Illinois Institute of Technology)
Closed-loop control of blood glucose concentration, known as artificial pancreas (AP) system, is an alternative treatment for patients with type 1 diabetes, by automatically controlling their blood glucose levels [1]–[2]. These control systems use continuous glucose measurements to calculate optimum amount of insulin to be infused with an insulin pump in order to keep plasma glucose concentration within a safe target range to avoid health problems. Real-time estimations for plasma insulin concentration is beneficial for increasing the efficiency of AP control algorithms. This enables calculation of more realistic insulin infusion rates and prevention of hypoglycemia that would be caused by over dosing of insulin.
Our objective is to fulfill a real-time estimation of plasma insulin concentration from continuous glucose monitoring data by using a mathematical model. Hovorka's model which has been developed to describe glucose-insulin dynamic in different parts of the human body, has been incorporated into a continuous-discrete extended Kalman filter (CDEKF) to provide an estimate of the plasma insulin concentration. The CDEKF is the generalization of the Kalman filter to nonlinear systems with continuous-time state equations and discrete-time measurements. Furthermore, because of variability in system dynamics, uncertain parameters have been considered as new states in Hovorka's model to be estimated by CDEKF.

This methodology has been evaluated by using clinical data from patients with Type 1 diabetes who underwent a closed-loop AP experiment. Real-time insulin estimations for two different cases which are with and without considering meal effects have been compared to plasma insulin measurements to evaluate performance and validity of the proposed methodology.
Finally, based on simulation results, it has been shown that the proposed method is able to estimate the plasma insulin concentration in real time. This method will be beneficial for an AP system in terms of real time estimation of non-measurable variables such as plasma glucose and insulin concentrations.
[1]. K. Turksoy, L. T. Quinn, E. Littlejohn, and A. Cinar, "An Integrated Multivariable Artificial Pancreas Control System," J. Diabetes Sci. Technol., vol. 8, no. 3, pp. 498–507, 2014.
[2]. K. Turksoy, L. Quinn, E. Littlejohn, and A. Cinar, "Multivariable Adaptive Identification and Control for Artificial Pancreas Systems," IEEE Trans. Biomed. Eng., vol. 61, no. 3, pp. 883–891, 2014.

10:25 AM **A Simulation Model Assessing the Integration of a Cold Thermal Energy Storage (TES) into an Air Conditioning System** (FrA1c)
Ahmed Aljehani, Said Al-Hallaj (University of Illinois at Chicago), *Siddique Khateeb* (AllCell Technologies)
Around the world, residential/commercial electricity consumers pay higher electricity prices during (peak hours) to air condition (cool) their spaces. Here in the US, some utilities companies in multiple states charge additional $0.05-0.07/ kWh (on average) during peak hours. The same analogy can be seen around the globe at even higher proportions. Furthermore, in some developing countries, utilities companies cannot even meet the peak hour's demand resulting in electricity delivery interruptions in some parts of the city. Thus, a demand side management initiatives came into play in the US and the rest of the world. Having said so, a thermal energy storage (TES) using a phase change composite (PCC) material, can be integrated with the refrigerant cycle of the air conditioning (A/C) system to shave the load during peak hours. In principle, the A/C's refrigerant cycle during (off peak hours) can be routed through a PCC exchanger to store coolness during the night, where electricity prices are "low". The PCC material will undergo a phase change from liquid to Solid, rejecting the heat to the refrigerant loop. Storing coolness in the PCC exchanger is commonly known as the "charging phase". On the other hand, during peak hours, hot circulated air from the space, which requires cooling, will be routed through the PCC exchanger system. At this case, the hot air will exchange heat with an intermediate refrigerant loop that passes the heat load into the PCC material. Accordingly, PCC absorbs the heat load and encounters a phase change from solid to liquid, which is commonly known as the "Discharging Phase". The amount of energy stored or released by the PCC is equivalent to the latent heat of the composite. Accordingly, a system analysis using Aspen Plus simulation was executed interconnecting the four main elements of the proposed system (Air load "stream", A/C refrigerant "loop", PCC exchanger and the intermediate refrigerant "loop") during charging and discharging phases. The preliminary results showed that a new A/C system coupled with a TES will require a smaller refrigerant compressor and smaller refrigerant loop (reducing initial capital cost), fewer Co2 emissions (better for the environment) and less electricity consumptions during peak hours (cost savings on electricity prices for consumers) and lower electricity demand during peak hours (reducing the necessity for utilities companies to build more plants to generate more electricity that only used during peak hours) and increasing the efficiency of the refrigerant compressor. The charging/discharging rates for the PCC material are extracted from the real experiment set up performed by All Cell Technologies group and fed into this simulation. A parallel paper addressing the experimental part and results was also submitted, by All Cell Technologies group, to participate on this respected conference.

10:45 AM **Population Balance Modeling of Mechanical Dispersion of semi-solid binders in High Shear Wet Granulation** (FrA1d)
Sudarshan Ganesh, Nathan J. Davis, James D. Litster (Purdue University)
An important unit operation in manufacture of dry laundry detergent powders is high shear wet granulation. High shear wet granulation is a process in which fine powders combine with a liquid binder to produce granules. Compared to the fine powders, the product granules are easy to handle, flow better and create less dust. The binder used in dry laundry detergent manufacture is a semi-solid surfactant blend. The surfactant binder does not penetrate the powder bed by capillary action producing an infinite drop penetration time irrespective of the dimensionless spray flux. This material property requires the granulation of semi-solid binders to operate in the mechanical dispersion region of the nucleation regime map.
This study builds on the pervious experimental work of mechanical dispersion for two paste blends in a pin mixer. The previous study examined the effects of impeller RPM and the paste injection temperature on the particle size distribution of the surfactant granule nuclei. In this study the mechanical dispersion of the binder is modeled as a breakage process using a 1D breakage only population balance model. The breakage kernel for the population balance model involves the selection function and the breakage distribution function, which describe the breakage probability of a particle and the distribution of the particle into its daughter particle respectively. The full particle size distributions are analyzed for parameter estimation using gSOLIDS (Process Systems Enterprise-Advanced Process Modelling of Solids Processes) with the built in Vogel and Peukert [1] breakage probability model and a power law breakage distribution function. A modified paste breakage selection function is being derived from the Vogel

and Peukert model, based on understanding of granulation processes.

The breakage kernel includes the inputs from material properties and operating conditions. The particle size distribution of a binder (Paste A) is analyzed for parameter estimation at a certain operating condition. The size distribution at different operating conditions for Paste A is then predicted by adjusting the parameters by physical understanding of the process and compared with the experimental data. Using the model operating parameters, a parameter estimation is done for the material parameters for a different paste (Paste B) at one set of conditions. These parameters are then adjusted based on operating conditions to predict the size distribution of Paste B. The model size distributions are compared with the experimental size distributions and the two distributions are statistically analyzed for similarity.

The Vogel and Peukert breakage selection model, derived for brittle material breakage is being modified for semi-solid material breakage. The paste breakage model is shown to be predictive for nucleation by mechanical dispersion.

[1]. L. Vogel, W. Peukert, From single particle impact behaviour to modelling of impact mills, Chem. Eng. Sci. 60 (2005) 5164–5176. doi:10.1016/j.ces.2005.03.064.

11:05 AM **Modeling and Optimization of Spherical Crystallization through a Coupled Population Balance Framework** (FrA1e)

Ramon Pena, Zoltan K. Nagy, Doraiswami Ramkrishna (Purdue University), *Christopher L. Burcham, Daniel J. Jarmer* (Eli Lilly & Co.)

Since its introduction by Randolph and Larson[1] (1971) and the solution methods described by Ramkrishna[2] (2000), the population balance model (PBM) has been widely used and accepted as model formulation method for simulation and prediction of the size distribution and other properties of particulate systems. PBMs allow for systems that include any or all of the following mechanisms: nucleation, growth, breakage and agglomeration. Following the initial work by Smoluchowski[3] (1917) on the rate of aggregation for spherical particles, there have many contributions for systems that exhibit agglomeration including dispersion (bubble) coalescence[4,5], granulation[6,7] and particle aggregation during crystallization[8,9,10]. The commonality in the limitations of many of the previous studies were physically irrelevant and/or empirically based agglomeration kernels, difficulty in assessing the influence of process conditions (e.g. hydrodynamics, particulate physical properties), solution method efficiency for optimization and control applications, and loss of information of constituent particles. These limitations present obstacles for the simulation, optimization, and control of the increasingly popular agglomeration technique of spherical crystallization.

Peña and Nagy[11] studied and showed the benefits of spherical crystallization as a process intensification technique whereby both internal (primary crystals) and external (agglomerates) properties can be controlled experimentally through a decoupled continuous spherical crystallization (CSC) approach; providing the means by which both biopharmaceutical (bioavailability, dissolution) and manufacturing (flowability, filtration, drying) properties can be simultaneously adapted to meet desired quality specifications. This technique opens the door for combined experimental and modeling approaches for the optimization and control of both the primary crystal and agglomerate properties in spherical crystallization processes. However, many of the PBMs currently in literature would fail to accomplish this because of the aforementioned limitations and loss of information.

To overcome the issues of loss information a coupled PBM formulation is required. A coupled PBM formulation could simultaneously track the evolution in the primary crystals and the evolution of the agglomerates. The relationship between primary crystal properties and their effect on final agglomerate properties would thereby be more evident and more efficient than traditional approaches. To the best of our knowledge, the only previous work that presented this approach is that of Ochsenbein et al.[12]. In their study, Ochsenbein et al.[12] focused on the agglomeration of needle-like crystals in suspension. Through a coupled PBM framework Ochsenbein et al.[12] were able to develop a population balance equation (PBE) to describe the evolution of the primary crystals by a two-dimensional growth rate to represent the needle like structure of the crystal. They then used another PBE to describe the evolution of the agglomerates as a function of the primary crystals. For the agglomeration kernel, they derived their own modified kernel that include both characteristic lengths of the primary crystals participating in the agglomeration. The new PBM formulation also allowed for the development of new parameters that add value to the simulations due to their experimental relevance. However, the work of Ochsenbein et al.[12] neglected nucleation something common to previously developed agglomeration models. The coupled population balance model framework will be extended herein.

The contribution of this work is the extension of the coupled PBM framework for application in the simulation and optimization of a spherical crystallization system. A coupled PBM framework has been developed for a semi-batch, reverse addition, anti-solvent crystallization system with agglomeration. The system includes nucleation and growth the primary crystals and subsequent agglomeration. The purpose of the work is to exploit the advantages presented by a coupled PBM framework; for example, the ability to optimize for specific primary and agglomerate sizes. This presents an opportunity to find optimal operating conditions that meet both bioavailability and manufacturability demands. It also allows for the ability to develop first principles based parameters for agglomeration efficiency and porosity. Additionally, through the retention of the information of the primary particles the interplay between the effects of operating conditions on the properties of the primary crystals versus the agglomerates will be clear.

1. Randolph, A.; Larson, M. Theory of particulate processes; analysis and techniques of continuous crystallization. 1971. New York: Academic Press.
2. Ramkrishna, D. Population balances theory and applications to particulate systems in engineering. 2000. San Diego, CA: Academic Press.
3. Smoluchowski, M. V. Z. Physical Chemistry, 1917, 19, 129–168.
4. C. a. Coulaloglou and L. L. Tavlarides. Description of interaction processes in agitated liquid-liquid dispersions. Chemical Engineering Science, 1977, 32(11), 1289–1297.
5. M. J. Prince and H. Blanch. W. Bubble coalescence and break-up in air-sparged bubble columns. AIChE Journal. 1990, 36(10), 1485–1499.
6. Simon M. Iveson. Limitations of one-dimensional population balance models of wet granulation processes. Powder Technology, 2002, 124(3), 219-229.
7. L. X. Liu and J. D. Litster. Population balance modelling of granulation with a physically based coalescence kernel. Chemical Engineering Science, 2002, 57(12), 2183-2191.
8. P. Marchal, R. David, J.P. Klein, and J. Villermaux. Crystallization and precipitation engineering—I. An efficient method for solving population balance in crystallization with agglomeration. Chemical Engineering Science, 1988, 43, 59–67.
9. R. David, P. Marchal, J.P. Klein, and J.V. Klein. Crystallization and Precipitation Engineering III. A Discrete Formulation of the Agglomeration Rate of Crystals in a Crystallization Process. Chemical Engineering Science, 1990, 46(1), 205–213.
10. Sanjeev Kumar, D. Ramkrishna, On the solution of population balance equations by discretization—III. Nucleation, growth and aggregation of particles. Chemical Engineering Science, 1997, 52(24), 4659-4679.
11. R. Peña and Z. K. Nagy. Process Intensification through Continuous Spherical Crystallization Using a Two-Stage Mixed Suspension Mixed Product Removal (MSMPR) System. Crystal Growth & Design, 2015, 15(9), 4225-4236.
12. D.R. Ochsenbein, T. Vetter, S. Schorsch, M. Morari, and M. Mazzotti. Agglomeration of Needle-like Crystals in Suspension: I. Measurements. Crystal Growth & Design, 2015, 15(4), 1923–1933.

Tissue Engineering I

Friday, March 4, 2016 (Armour Dining, **FrA2**)
Chair: *Nancy Karuri* (Illinois Institute of Technology)
Co-Chair: *Ashty Karim* (Northwestern University)

9:45 AM **Effect of Fibronectin on the Diffusion and Rigidity of the Fibrin-Fibronectin Matrix** (FrA2a)
Chengyao Wang, Nancy W. Karuri (Illinois Institute of Technology)

The fibrin-fibronectin (FbFn) matrix is a scaffold for tissue development during wound healing and has been used extensively in tissue engineering and drug delivery. While the influence of fibrin concentration has been well studied and documented on FbFn matrix properties, the role of fibronectin concentration is not clearly understood. Our lab had previously demonstrated that fibronectin levels influence the structural characteristics of FbFn matrix. To address the question whether fibronectin concentration had an effect on (i) the elasticity of, and (ii) diffusion in the FbFn matrix, we measured the elastic modulus and diffusion coefficient of FbFn matrices with different amounts of fibrin and fibronectin. The former was measured by compression studies in a rheometer and the latter was determined by Fluorescence Recovery After Photobleaching (FRAP) measurements of 40kDa dextran-fluorescein in reconstituted matrices made from 0-0.4 mg/ml human plasma fibronectin and 2 mg/ml and 4 mg/ml fibrinogen solutions. FbFn matrices made with 4 mg/ml fibrinogen had a higher elastic modulus and higher diffusion coefficient than matrices made from 2 mg/ml. Our results revealed that the elastic modulus decreased from 2330 N/m^2 to 1925 N/m^2 when fibronectin concentration increased from 0 mg/ml to 0.4 mg/ml in matrices made with 4 mg/ml fibrinogen, whereas the diffusion coefficient decreased from 5.5 $x10^{-6}$ cm^2/s to 4.5 $x10^{-6}$ cm^2/s. These findings are novel and support previous studies from our laboratory showing that elevated fibronectin concentrations lead to shorter and less dense matrix fibers. They also provide a foundation for in vitro studies of tissue development with FbFn matrices.

10:05 AM **MR Tools for the Assessment of Cartilage and Osteochondral Tissue Engineering** (FrA2b)
Mrignayani Kotecha (University of Illinois at Chicago)

Cartilage and osteochondral tissue engineering is an active field of research for the past three decades. Cartilage tissue engineering uses a combination of biomaterial, cells and growth factors to achieve a neocartilage tissue that can be used for providing permanent cure to cartilage damage caused by osteoarthritis, trauma or developmental issues. After initial success at-bench, most tissue growth strategies are tested in animal models before they can reach to patients. However, most successful preclinical tissue engineering approaches do not scale up to clinics. In many cases, these tissues do not measure upto the functional challenges of load bearing joints. A key technical challenge is the functional assessment of engineered tissues, pre and post-implantation. Magnetic resonance spectroscopy (MRS) and magnetic resonance imaging (MRI) are leading non-invasive techniques in assessing the growth of cartilage regeneration (1-8). MR techniques provide an unparalleled amount of information of tissue microstructure, extracellular matrix amount, cellular activities, molecular dynamics and tissue anisotropy. Thus, we have an opportunity to use MR for guiding successful tissue engineering. In this presentation, I will discuss advances made in MR assessment of tissue-engineered cartilage and osteochondral tissues in our group, as well as challenges and opportunities in the near future.

[1]. Ravindran S, Gao Q, Kotecha M, Magin RL, Karol S, Bedran-Russo A, et al. Biomimetic Extracellular Matrix-Incorporated

Scaffold Induces Osteogenic Gene Expression in Human Marrow Stromal Cells. Tissue Eng Part A. 2012;18(3-4):295-309.
[2]. Kotecha M*, Ravindran S, Schmid TM, Vaidyanathan A, George A, Magin RL. Application of sodium triple-quantum coherence NMR spectroscopy for the study of growth dynamics in cartilage tissue engineering. NMR in biomedicine. 2013;26(6):709-717.
[3]. Kotecha M*, Klatt D, Magin RL. Monitoring cartilage tissue engineering using magnetic resonance spectroscopy, imaging, and elastography. Tissue Engineering Part B. 2013;19(6):470-484.
[4]. Kotecha M*, Schmid TM, Odintsov B, Magin R. Reduction of water diffusion coefficient with increased engineered cartilage matrix growth observed using MRI. Engineering in Medicine and Biology Society (EMBC), 2014 36th Annual International Conference of the IEEE. 3913 - 3916.
[5]. Pothirajan P, Dorcemus DL, Nukavarapu S, Kotecha M*. True MRI assessment of stem cell chondrogenesis in a tissue engineered matrix. Engineering in Medicine and Biology Society (EMBC), 2014 36th Annual International Conference of the IEEE. 3933- 3936.
[6]. Pothirajan P, Ravindran S, George A, Magin R, Kotecha M*. Magnetic resonance spectroscopy and imaging can differentiate between engineered bone and engineered cartilage. Engineering in Medicine and Biology Society (EMBC), 2014 36th Annual International Conference of the IEEE. 3929-3932.
[7]. Ravindran S, Kotecha M, Huang C-C, Ye A, Pothirajan P, Yin Z, et al. Biological and MRI Characterization of Biomimetic ECM Scaffolds for Cartilage Tissue Regeneration. Biomaterials. 2015;71:58-70.
[8]. Majumdar S, Pothirajan P, Dorcemus D, Nukavarapu S, Kotecha M*. High Field Sodium MRI Assessment of Stem Cell Chondrogenesis in a Tissue-Engineered Matrix. Annals of Biomedical Engineering. 2015: in press.

10:25 AM **Agent-Based Modeling of Scaffold Vascularization and Bone Tissue Regeneration Using Biodegradable Polymer/Ceramic Composite** (FrA2c)

Chenlin Lu, Elif S. Bayrak, Mustafa C. Ozturk, Banu Akar, Eric M. Brey, Ali Cinar (Illinois Institute of Technology)

A variety of bioactive composite materials have been investigated over the past two decades for angiogenesis and tissue regeneration. Biodegradable biomaterial scaffolds are often combined with calcium phosphates, such as hydroxylapatite (HA) and tricalcium phosphate (TCP) to serve as good substrates for bone tissue engineering. Biomaterial scaffolds provide essential mechanical and structural support for scaffold vascularization and appropriate cell function and morphogenesis, whereas the ceramics have high biocompatibility and osteoinductivity. Interaction between blood vessel formation, bone cell growth and modified biomaterial structure are often difficult to study with experimentation alone. Therefore, an agent-based computational model (ABM) was developed to investigate vascularization and bone tissue regeneration in a biodegradable, porous hydrogel/calcium phosphate biomaterial composite.

Two previously developed agent-based models (ABM) in our research group, one described the biomaterial scaffold vascularization [1] and the other described bone tissue regeneration [2], were combined together to investigate the comprehensive process. A statistical model developed by Metters et al. to describe the bulk degradation of PLA-b-PEG-b-PLA hydrogel is applied to incorporate scaffold degradation factors into the model [3]. The modified ABM is focused on the combined effects of scaffold vascularization and ceramic incorporation on bone tissue regeneration.

The simulation results indicate that calcium phosphates play an important role in bone tissue regeneration due to their osteoinductivity. Scaffold vascularization is another important factor for bone tissue regeneration and it can be enhanced by modifying the degradation characteristic of scaffolds. Simulations show the flexibility of the developed ABM and exemplify the types of investigation it enables. These results can be used in combination with experimental research to design optimal scaffold structures.

[1]. H. Mehdizadeh, S. Somo, 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]. E.S. Bayrak, H. Mehdizadeh, B. Akar, S. Somo, E.M. Brey, A. Cinar “Agent-based modeling of osteogenic differentiation of mesenchymal stem cells in porous biomaterials.” EMBC, August 2014.
[3]. 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.

10:45 AM **Synthesis and Characterization and In-Vivo Efficacy of a Lubricin Mimic to Reduce Progression of Osteoarthritis** (FrA2d)

Jim McMasters, Alyssa Panitch, Shaili Sharma (Purdue University), *Corey P. Neu* (University of Colorado, Boulder), *Alexandra Lawrence* (Biomet)

The proteoglycan, lubricin, facilitates the remarkable low friction and wear properties of articular cartilage in the synovial joints of the body. Decreased expression of lubricin is associated with cartilage degradation and the pathogenesis of osteoarthritis. Development of therapeutic molecules that mimic lubricin function remains a need for early osteoarthritis treatment. We engineered a lubricin mimic (mLub) that is less susceptible to enzymatic degradation and binds to the articular surface to reduce friction. mLub was synthesized using a chondroitin sulfate backbone with type II collagen and hyaluronic acid (HA) binding peptides to promote interaction with both the articular surface and synovial fluid constituents. In vitro and in vivo characterization confirmed the binding ability of mLub to isolated type II collagen and HA, and to the cartilage surface. Further in vivo studies demonstrated the ability of mLub to attenuate the progression of OA. Using an ex vivo model of damaged cartilage, application of mLub, in combination with purified or commercially available hyaluronan, reduced the coefficient of friction, and adhesion, to control levels. In vivo studies demonstrated a mLub residency time of less than 1 week, and analysis of overall joint health showed that mLub treatment reduced cartilage degradation. Enhanced lubrication by mLub reduces surface friction and adhesion, which may be the factor contributing to the suppressed progression of degradation and cartilage loss in the joint. mLub therefore shows potential for treatment in early osteoarthritis following injury.

11:05 AM **Manipulating Focal Adhesion Formation by Nanotopographical Substrates for Enhanced Myogenic Differentiation of Primary Myoblasts** (FrA2e)
Eunkyung Ko, Hyunjoon Kong (University of Illinois at Urbana-Champaign), *Seung-Jung Yu, Sung Gap Im* (Korea Advanced Institute of Science and Technology)
Myogenic commitment of stem cells and primary myoblasts has drawn attention for developing treatments for skeletal muscle diseases. Biophysical cues as well as biochemical cues are known to influence the cellular mechanism of the myogenic differentiation event. Recent studies have revealed that among the biophysical signals, topography can manipulate cellular functions by guiding the focal adhesions of cells. Substrates with nano and micro scale grooves and ridges have been shown to cause contact guidance of cells, thereby, enhancing the cellular responses. In this study, we developed a nano scale line-patterned substrate ranging from 200 to 1600 nm to investigate the topographical effect on the primary myoblasts focal adhesion, alignment, and differentiation. Primary myoblasts cultured on the line patterns showed better alignment in their morphology and expressed more muscle differentiation markers. Muscle contraction of the cells cultured on the line patterned substrates was occurring in an isotropic manner which resulted in higher contraction frequency compared to the cells cultured on an unpatterned substrate. Lastly, we engineered a neuromuscular junction on the cultured muscle cell layer to analyze how topography can influence neuromuscular junction formation and muscle contraction.

Refining and Petrochemical Engineering I
Friday, March 4, 2016 (Alumni Lounge, **FrA3**)
Chair: *Paolo Palmas* (UOP/Honeywell)
Co-Chair: *Emad Ghadirian* (Illinois Institute of Technology)

9:45 AM **Maximizing Diesel Production in an FCC Refinery** (FrA3a)
Ron Subris (UOP/Honeywell)

- FCC based refinery will face challenging situation to meet the growing diesel demand
- New developments to increase the quality and quantity of the light cycle oil (LCO) from the FCC unit to enable a greater proportion of LCO to be blended into the refinery's distillate pool
- New technologies to allow use of FCC and refinery light olefin streams for diesel production.
- Case studies illustrating each of these advancements and the value they can bring to a US-based FCC refinery will be presented

10:05 AM **Numerical Simulation of an Industrial Fluid Catalytic Cracking Regenerator** (FrA3b)
Chenn Zhou, Bin Wu, Guangwu Tang, Armin Silaen (Purdue University - Calumet)
Fluid catalytic cracking (FCC) is one of the most important conversion processes in petroleum refineries, and FCC regenerator is a key part of an FCC unit to recover the solid catalyst activity by burning off the deposited coke on the catalyst surface. In modern FCC units, regenerator is a cylindrical vessel. Carrier gas transports the solid catalyst from the stripper and feeds the catalyst into the regenerator through catalyst distributors. The catalyst is fluidized by the air that is injected into the regenerator through air rings in the bottom part of the cylindrical vessel. A three-dimensional multi-phase, multi-species reacting flow computational fluid dynamics (CFD) model was established to simulate the flow inside an FCC regenerator. The two phases involved in the flow are gas phase and solid phase. The Euler-Euler approach, where the two phases are considered to be continuous and fully inter-penetrating, is employed. The model includes gas-solid momentum exchange, gas-solid heat exchange, gas-solid mass exchange, and chemical reactions. Chemical reactions incorporated into the model simulate the combustion of coke which is present on the catalyst surface. The simulation results show a good agreement with plant data.

10:25 AM **Improving Refinery Unit Start-ups and Shut Downs** (FrA3c)
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 **Dividing-Wall Column Screening Guidelines and Applications** (FrA3d)
Robert Tsai, Paul Steacy, Xin X. (Frank) Zhu (UOP/Honeywell)

A dividing-wall column (DWC) is a distillation column with a vertical partition that can be implemented as a potentially attractive alternative to conventional multi-column or sidecut column arrangements; use of a DWC may enable capital cost and energy savings of around 30% or even higher to be achieved. Rules-of-thumb involving process conditions like feed composition and relative volatility are often cited for consideration when trying to determine if a DWC might make sense (or not) in a given flowscheme. The intent of this work is to present and review these guidelines in the context of refining and petrochemical processes and obtain an updated perspective that will allow for more detailed guidance to be provided for future screening evaluations.

11:05 AM **Performance of Petrochemical Buildings Subject to Fire Hazards** (FrA3e)
Ernesto Gasulla (Baker Risk Engineering and Risk Consultants, Inc.)

Abstract: Fire is the most common hazard to personnel in petrochemical plants. While the thermal characteristics of a building or parts of it are often expressed in terms of "One Hour Resistant" or similar, the definition of thermal resistance is more complex than that. As a result, buildings commonly deemed as "Fire Resistant" may not perform adequately in the event of a fire. This presentation will discuss the different types of fires commonly found in a plant (jet and pool fires), codes and regulations related to thermal performance of buildings (ASTM E119 & E1529, NFPA 80, NPD Classes, etc.), and criteria used to evaluate the adequacy of a building to fire exposure. Design cases based on thermal performance software models (Fire Dynamic Simulator) shall be presented and discussed.

<u>**Environmental Engineering**</u>
Friday, March 4, 2016 (Herman Lounge, **FrA4**)
Chair: *Gerardo J. Ruiz-Mercado* (U.S. EPA)
Co-Chair: *Jarad L. Champion* (Geosyntec Consultants)

9:45 AM **Improving Resource Availability for Sustainable Manufacturing: Review and Case Study on Phosphorus** (FrA4a)
Daniel Bampoh, Shweta Singh (Purdue University)

Resource limitations are a serious threat to sustainable manufacturing especially when there are no substitutes. Phosphorus (P) is one of the critical element for sustainability as it forms the major constituent for food production and other industrial manufacturing. As global demand for phosphorus rises exponentially to meet the food demand, known phosphorous reserves are estimated to run out which will also jeopardize other manufacturing activities dependent on P. There are opportunities to recover phosphorous from existing municipal, industrial and agricultural waste streams, and the European Union is leading several efforts in the development and application of P-recovery technologies to meet this challenge with P-recycling rates as high as 53% in some countries. The US is comparatively underachieving in this light. It is important that the US and other countries also play a significant role in addressing phosphorous loss by adopting, disseminating and exploring P-recovery methodologies for enhanced P-use efficiency. In this work, we provide a review of P recovery technologies and assess the potential of adopting two recovery technologies within US through life cycle assessment. Results indicate that struvite crystallization technology modules attached to US wastewater treatment plants would recover 7% more P but with an average of 10% more environmental impacts on an average order of 109 kg-emissions-eq. Prospects indicate there are opportunities to recover a collective 2 million to 3 million tons of phosphorus from US waste streams.

10:05 AM **Electrochemical Impedance Spectroscopy Study of Membrane Fouling and Electrochemical Regeneration at a sub-Stoichiometric TiO2 Reactive Electrochemical Membrane** (FrA4b)
Yin Jing, Lun Guo, Brian P. Chaplin (University of Illinois at Chicago)

Membrane fouling increases operational cost and reduces membrane life, which is not easily understood by current methods. Traditional chemical cleaning method is not cost effective or environmentally friendly. In this study, a non-invasive and non-destructive electrochemical impedance spectroscopy (EIS) characterization method was adopted to study membrane fouling at a novel reactive electrochemical membrane (REM). The REM consists of a porous substoichiometric titanium dioxide tubular ceramic electrode operated in the cross-flow filtration mode. Theoretical Transmission Line Model was successfully developed to interpret EIS results. Based on the spatial study of membrane fouling by model foulants humic acid and polystyrene microspheres, a chemical free electrochemical regeneration method in backwash mode was established. Through this method, the flux of a fouled REM was able to recover from 3% to between 76% and 99% of the initial over 5 continuous fouling/regeneration cycles in the case of humic acid fouling and full recovery in that of polystyrene microsphere fouling. Besides, the operating cost of this method is much more competitive and is only 1.3% of that of NaOH cleaning. Results illustrate the promising future of the REM which allows it to function in a diverse set of water treatment applications.

10:25 AM **Detecting Heavy Metals in Water using Carbon Nanotube Threads** (FrA4c)
David Siebold, Vesselin Shanov, William R. Heineman, Noe Alvarez, Daoli Zhao (University of Cincinnati)

Carbon nanotube (CNT) threads inherit the advantages of CNTs, while avoiding the potential toxicity caused by individual CNTs. Electrodes based on CNT threads were fabricated and used for simultaneous detection of trace levels of heavy metal ions by anodic stripping voltammetry (ASV). The operational parameters such as deposition potential and deposition time were optimized in 0.1 M acetate buffer solution (pH = 4.5). The CNT thread electrode gives well-defined, reproducible and sharp stripping signals for individual and simultaneous detection of heavy metals ions. The detection limits are far below the requirement of WHO in water.

10:45 AM **Removal of Phenol from Produced Water Utilizing a NiO-based Catalyst in Supercritical Water** (FrA4d)
Chamara De Silva, Jason Trembly (Ohio University)

The U.S. oil/gas industry generates over 21 billion barrels of produced water annually [1]. This waste water stream contains a host of components including suspended solids, dissolved solids, and hydrocarbons and could be reused in beneficial applications to reduce water demands [2]. However, many beneficial reuse applications have strict hydrocarbon limits [3]. With the support from the Research Partnership to Secure Energy for America, Ohio University is developing a produced water treatment process which takes advantage of supercritical water properties to remove both dissolved solids and hydrocarbons. To quickly and effectively remove hydrocarbons in supercritical water a heterogeneous catalyst is required. In is study, a NiO/Al2O3 catalyst was synthesized, characterized and evaluated for phenol removal performance in supercritical water. Synthesized catalysts were characterized using temperature programmed reduction, pulse chemisorption, x-ray powder diffraction and scanning electron microscopy with energy dispersive x-ray spectroscopy. Catalyst activity for phenol conversion was evaluated in a continuous packed bed reactor at supercritical water conditions, while analyzing liquid and vapor products. Process variables evaluated included free O2 to carbon ratio, temperature and residence time. Results from the NiO/Al2O3 catalyst study, including catalyst characterization and performance results, will be presented.

[1]. J. Veil, "U.S. Produced Water Volumes and Management Practices in 2012," Ground Water Protection Council, Apr. 2015.

[2]. T. Hayes, "Sampling and Analysis of Water Streams Associated with the Development of Marcellus Shale Gas," Marcellus Shale Coalition, Des Plaines, IL, Dec. 2009.

[3]. C. W. Abdalla, J. R. Drohan, K. S. Blunk and J. Edson, "Marcellus Shale Wastewater Issues in Pennsylvania," The Pennsylvania State University, 2015.

11:05 AM **Design of Novel Polymeric Adsorbents for Metal Ion Removal from Water Using CAMD** (FrA4e)
Urmila Diwekar, Rajib Mukherjee, Berhane Gebreslassie (Vishwamitra Research Institute)

Heavy metals acts as contaminants in drinking water. They are generally removed from drinking water using cation exchange resins. Resins act as an adsorbent of the heavy metals. Chelating resins are generally available commercially with limited adsorption capacity. Manufacturing novel resins polymers for enhanced adsorption of metal ion requires ample experimental efforts that are expensive as well as time consuming. To overcome these difficulties, application of computer-aided molecular design (CAMD) will be an efficient way to develop new chelating resin polymers. In this effort CAMD based on group contribution method (GCM) has been used to design novel resins with enhanced capabilities to remove heavy metal ions from water. Polymers are consists of monomers with varied chain lengths. Each monomer unit of the polymer can be subdivided into different structural and functional groups. The adsorption mechanism depends on the difference in activities of the heavy metals in adsorbents and the bulk fluid phase. In the present work, different chelating resin polymers used for adsorption are subdivided into structural and functional groups. The activity coefficient of heavy metal in the solid phase and bulk phase is estimated using a modified version of the UNIFAC group contribution method. The contribution of the functional groups in the adsorption process are then used in a combinatorial optimization method for computer aided molecular design of novel resin polymers. The designed polymer has an order of magnitude higher adsorption capacity compared to conventional resin used for the same purpose.

Keywords: chelating resin, heavy metal ions, group contribution method (GCM), adsorbate-solid solution theory (ASST), computer-aided molecular design (CAMD), efficient ant colony optimization (EACO)

<u>Fluid Properties and Transport Phenomena</u>

Friday, March 4, 2016 (Crown Room, **FrA5**)
Chair: *Lewis Wedgewood* (University of Illinois at Chicago)
Co-Chair: *Joseph Whittenberg* (University of Illinois at Urbana-Champaign)

9:45 AM **Microfluidic Mixing to Prepare Polyaspartamide Nanoparticles** (FrA5a)
Nicholas E. Clay, Joseph J. Whittenberg, Vivek Kumar, Jinrong Chen, Paul Kenis, Hyunjoon Kong (University of Illinois at Urbana-Champaign)

In the past two decades, polymersomes and micelles have been widely studied for a variety of applications, including in vivo drug delivery, bioimaging, microreactions, and sensors. These polymeric nanoparticles are prepared from an amphiphilic polymer through either solvent-free or solvent-exchange methods. Despite the advancements made in nanoparticle technology, widespread industrial adoption is limited in part due to poor size control, challenging amphiphilic polymer synthesis, and low molecular encapsulation efficiency. To meet this challenge, we sought to investigate the role that mixing rate and molecular solubility played on the controlled assembly of micelles and polymersomes. To control mixing rate, we conducted nanoparticle synthesis in a flow-focusing microfluidic device. We first prepared a polyaspartamide-based polymer grafted with octadecyl chains and valine groups (termed "PHEA-C18-val"). The octadecyl groups gave PHEA-C18-val a strong hydrophobic character, while the valine groups improved solubility in dimethylformamide (the "cosolvent phase"). Two different PHEA-C18-val polymers were produced, with a degree of substitution of the octadecyl chain (DS-C18) of approximately 20 % and 40 %, respectively. By gradually removing the cosolvent phase via laminar mixing on the microfluidic chip, different PHEA-C18-val (DS-C18 20 %) micelle sizes could be created, ranging from 100 to 200 nm. Separately, micelles were prepared via off-chip drop-wise precipitation, with a size around 300 nm. All micelles had a polydispersity index below 0.2, suggesting a good degree of size control. With off-chip precipitation, stable PHEA-C18-val (DS-C18 40 %) polymersomes were formed, with a size around 100 nm and a bilayer thickness of 20 nm. Interestingly enough, no stable polymersomes were formed on-chip, as the polymer precipitated out before nanoparticle assembly was possible. To our knowledge, this project represents one of the first attempts to examine the combined effects of processing techniques and molecular solubility when preparing polyaspartamide nanoparticles. This process method reported herein will be broadly useful to improving the morphology and function of different nanoparticle systems.

10:05 AM **The Role of Additives and Orientation on the Gas Transport Properties of Poly (Ethylene Terephthalate)** (FrA5b)

Shahab Zekriardehani, Maria R. Coleman, Saleh A. Jabarin (University of Toledo)

Additives such as low molecular weight diluents (LMWD) can be added at low concentration to poly (ethylene terephthalate) (PET) to improve barrier properties significantly. Orientation during PET processing, on the other hand, causes strain induced crystallization which can increase the diffusion pathway and lessen the amorphous chain mobility. The objective of this work is to analyze the effect of LMWD additives, such as dimethyl terephthalate (DMT) and orientation on the free volume and thermal properties of PET and correlate this with barrier properties. Films of pure PET and PET/DMT made using single screw extruder were oriented using Long Extensional Tester at a relatively fast rate of 200%/s (4 in/s) to prevent any relaxations in the rubbery stage . TGA and FTIR were used to quantify concentration of DMT in the PET matrix. Permeation measurements were conducted using gases with different sizes (O_2, CO_2, CH_4, N_2, and He). Sorption measurements were performed to study the Langmuir and Henry's Law sorption sites in case of orientation and incorporation of low molecular weight diluents. Dynamic mechanical analysis (DMA) experiment was used to study long/short range chain motions. Besides, differential scanning calorimetry (DSC) was used to study the thermal properties and crystallinity. Transport studies demonstrated lower permeability for both oriented PET and PET/DMT samples, with the average barrier impact factors (BIF) of about 2 and 1.3 for all the gases, respectively. Sorption studies showed that both orientation and additive lessen the amount of Langmuir capacity constant (CH') which can be explained by the results from DMA and density measurements. The dynamic mechanical studies show more restriction in the chain motion in case of oriented PET and PET/DMT compared to unoriented PET. Furthermore, calculating fractional free volume using WLF equation offered lower values for oriented PET and PET/DMT compared to pure PET. Density measurement results also verified that orientation and additive lessen the amount of the free volume. However, the amount of the free volume calculated from both WLF equation and density measurements is lower for oriented PET than that of PET/DMT, which explains the lower permeability of oriented PET. DSC and density measurements results showed oriented PET has the highest level of crystallinity, about 30%, which is the result of strain induced crystallization during stretching oriented samples.

10:25 AM **Application of Non-uniform Magnetic Fields on Ferrofluid Colloidal Dispersions using an Iterative Constraint Method: A Brownian Dynamics Study** (FrA5c)

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

Ferrofluids are steadily rising in applications across many fields, preferred for their ability to be remotely positioned and controlled via external magnetic fields. Currently, most ferrofluid simulation techniques are focused on uniformly applied magnetic fields. The behavior of particles in ferromagnetic clusters in uniformly applied magnetic fields has been simulated using Brownian dynamics, Stokesian dynamics, and Monte Carlo methods. However, little research has been developed to observe the influence of non-uniformly applied magnetic fields in these simulations, especially at the particulate level. A constraint method is developed to satisfy Maxwell's Equations when a non-uniform magnetic field is applied to ferrofluids in a heterogeneous Brownian dynamics simulation that examines the effects of ferromagnetic clusters in a mesoscale particle collection. The procedure ensures that essential laws of magnetostatics are met, namely Maxwell's Equations. This is accomplished by allowing the system to advance by a time-step under a non-uniformly applied magnetic field, then adjusting the particles via an iterative constraint method until Maxwell's Equations are satisfied. Results are compared to existing Brownian dynamics simulations as well as homogeneous models, which assume magnetization is a direct effect of the magnetic field. In conclusion, the resultant constraint model, employed with the

Brownian dynamics technique, generates chain-like cluster formations and therefore, realistic ferrofluid behavior under a non-uniformly applied magnetic field while observing fundamental magnetostatic laws.

10:45 AM **Effects of Salt on the Stratification and Dynamics of Foam Films** (FrA5d)
Rabees Rafiq, Vivek Sharma, Subinuer Yilixiati (University of Illinois at Chicago)
The versatile intrinsic properties of liquid foams make them a crucial aspect of many industrial, biological, and cosmetic applications. Liquid foam films are colloidal dispersions of gas phase bubbles in a continuous liquid dispersion medium. The lifetime and stability of foams is related to the stratification, or step wise thinning, of the thin liquid film which separates two concurrent pockets of gas. The stratification of a micellar solution of various concentrations of sodium dodecyl sulfate with salt are examined through thin film thickness measurements in a Scheludko cell using a novel technique known as Interferometry Digital Optical Microscopy (IDIOM). The addition of salt to the surfactant solution results in a change in the step size of the stratification due to the increased shielding effect in the Stern Layer of the electrostatic double layer, a decrease in the characteristic thickness of the Guoy Chapman Layer (Debye Length) and a change in the packing parameter of the individual monomers. Though there have been previous studies focused on the stratification of liquid thin films, the effects of adding salt to the stratification and dynamics of thin films in a micellar solution has not received sufficient attention.

11:05 AM **Molecular Modeling of Isopropanol Dehydration Using Molecular Simulations in the Presence of Contaminants** (FrA5e)
Xiaoyu Wang, Sohail Murad (Illinois Institute of Technology)
NaA zeolite membranes are widely used for the dehydration of isopropanol. We have carried out molecular simulations to understand the molecular mechanisms, which make these membranes so efficient for dehydration. It has also been experimentally observed that the presence of hexane or acetone adversely affects the efficiency of the dehydration process. The precise reasons why this happens is not well understood. We have used molecular simulations to get a better understanding of this observed failure the molecular level. It our hope that with this improved understanding modifications can be made to the dehydration process to maintain their efficiency even when these contaminants are present.

__**Process Operations and Control**__
Friday, March 4, 2016 (Ballroom, **FrB1**)
Chair: *Alex Dowling* (University of Wisconsin)
Co-Chair: *Jin Zhang* (Illinois Institute of Technology)

2:00 PM **Optimal Control of Batch Distillation with Missing Components** (FrB1a)
Urmila Diwekar (Vishwamitra Research Institute)
Batch distillation is commonly used unit operation in specialty chemicals. In order to maximize the profitability and improve separation using batch distillation column, optimal reflux operation can be used. The mathematical and numerical complexities of the optimal control problem get worse when uncertainty is present in the formulation. However, in specialty chemical industries thermodynamic properties of not all chemical components of a mixture to be separated are known. These uncertainties in the problem formulation can result in sub-optimal solutions. These static thermodynamic uncertainties result in dynamic uncertainties due to unsteady state nature of batch distillation operation. In this work, we derive new optimality conditions based on Ito's lemma derived from financial literature where time dependent uncertainties are common. We use stochastic maximum principle for formulation of the resulting stochastic optimal control problem. This algorithm is implemented in the MultiBatchDS batch distillation process simulator. Finally, a numerical case-study derived from a real world batch distillation separation problem encountered at Firmenich is presented to show the scope and application of the proposed approach.

2:20 PM **Hybrid Online Sensor Error Detection and Functional Redundancy for Systems with Time-Varying Parameters** (FrB1b)
Jianyuan Feng, Kamuran Turksoy, Sediqeh Samadi, Iman Hajizadeh, Mert Sevil, Ali Cinar (Illinois Institute of Technology)
Supervision and control systems rely on signals from sensors to receive information to monitor the operation of a system and adjust manipulated variables to achieve the control objective. However, sensor performance is often limited by their working conditions and sensors may also be subjected to interference by other devices. Many different types of sensor errors such as outliers, missing values, drifts and corruption with noise may occur during process operations. Algorithms are needed to detect these errors, and replace the erroneous values with best estimates for use in supervision and control systems.
Methods:
A hybrid online sensor error detection and functional redundancy system is developed to detect errors in online signals, and replace erroneous or missing values detected with model-based estimates. The proposed hybrid system relies on two techniques, an outlier-robust Kalman filter (ORKF) and a locally-weighted partial least squares (LW-PLS) regression model, which leverage the advantages of automatic measurement error elimination with ORKF and data-driven prediction with LW-PLS. The system includes a novel method called nominal angle analysis to distinguish between signal faults and large changes in sensor values caused by real dynamic changes in process operation. The performance of the system is illustrated with clinical data generated by continuous

glucose monitoring (CGM) sensors from people with type 1 diabetes. More than 2000 CGM sensor errors were added to original CGM signals from 10 clinical experiments were analyzed for detection and analysis.
Results:
The results indicate that the sensor fault detection and data reconciliation system can successfully detect most of the erroneous signals and substitute them with reasonable estimated values computed by functional redundancy system. Correct error detection ranged from 70.9% to 97.4% for various types of sensor errors that lasted for 2-4 consecutive sensor readings. Successful reconciliation of glucose concentrations ranged from 81.9% to 98% for the same errors.

2:40 PM **Design of Dynamic Systems based on Efficient Ant Colony Optimal Control (EACOC) Algorithm: Case Study Chemical Process Control** (FrB1c)

Berhane H. Gebreslassie, Urmila M. Diwekar (Vishwamitra Research Institute), *Gaurav Mirlekar, Fernando V. Lima* (West Virginia University)

Many biological systems have shown success of solving difficult problems encountered in nature and hence, they have been source of inspiration for advanced control solution methods. For example, the behavior of the natural groups such as ants, bees and swarms demonstrates that self-organization and cooperation by following simple rules of interaction can result in a wide range of optimal patterns [1]. Inspired by ant's foraging behavior, the present work introduces a biomimetic optimal control strategy for chemical process control specifically for non-linear processes. The proposed strategy employs the computationally efficient optimal control solver entitled efficient ant colony optimal control (EACOC) algorithm. The EACOC algorithm is a metaheuristic optimization techniques inspired by the ants' foraging behavior which utilizes probabilistic and stochastic concepts for solving large scale optimization problems. A brief description of this algorithm is presented below.
In basic ant colony optimization (ACO) algorithm, artificial ants are stochastic candidate solution construction procedures that exploit a pheromone model and possibly available heuristic information of the mathematical model. The artificial pheromone trails are the sole means of communication among the artificial ants. Pheromone decay allows the artificial ants to forget the past history and focus on new promising search directions. The pheromone values are updated according to the information learned and hence, the algorithmic procedure leads to very good and hopefully, a global optimal solution. EACO algorithm improves the performance of the conventional ACO algorithm for combinatorial, continuous and mixed-variable optimization problems by introducing Hamersley sequence sampling (HSS) for probabilistic elements of ACO. The initial solution archive diversity for continuous and mixed-variable optimization problems plays an important role in the performance of ACO algorithm. The uniformity property of the HSS technique is exploited to avoid clustering of the initial solution archive in a small region of the potential solution space. Moreover, ACO algorithm is a probabilistic method where several randomized probability functions are involved in the algorithm procedure. The distribution of these random numbers affects the performance of the ACO algorithm. At this step, the multidimensional uniformity property of HSS is also introduced to improve the computational efficiency of the ACO algorithm. The capabilities of the proposed methodology are illustrated using benchmark problems and a real world case study of computer aided molecular design problem. Specifically, the problem is design of an optimal solvent for extraction of acetic acid from waste process stream using liquid-liquid extraction [3].
The EACOC algorithm is developed based on the efficient ant colony algorithm and orthogonal collocation methods. The proposed algorithm is implemented for optimal design of dynamic fermentation process where the objective function is tracking the product concentration set-point. The challenges in this fermentation process are the steady-state multiplicity and the oscillations in the concentration profile [2]. This approach successfully overcomes these challenges. The results show improvement in the solution quality and reduction computational time. The proposed algorithm can be used as an alternative to the gradient based optimal control algorithms for optimization of large scale dynamic problems.

[1]. Hristu-Varsakelis D. and Shao C. "A bio-inspired pursuit strategy for optimal control with partially constraints final state". Automatica 2007; 43:1265-1273.
[2]. Sridhar L. "Elimination of oscillations in Fermentation Process". AIChE Journal 2011;57(9):2397-2405.
[3]. Gebreslassie BH, and Diwekar UM. Efficient ant colony optimization (EACO) for computer aided molecular design: Case study solvent selection problem. Computers and Chemical Engineering 2015: 78: 1-9.

3:00 PM **Mixed-Integer Programming Solution Methods for Inventory Routing Problems** (FrB1d)

Yachao Dong, Chirstos T. Maravelias (University of Wisconsin Madison), *Jose M. Pinto, Arul Sundaramoorthy* (Praxair, Inc.)

To reduce the distribution cost in supply chains (SCs), vendor managed inventory (VMI) policy is adopted in many chemical industries. Under this policy, the vendor can decide when and how much to serve each customer, on the condition that the inventories of customers are kept between the agreed minimum and maximum levels. To make the distribution decisions under a VMI policy, the inventory routing problem (IRP) needs to be solved, in which the vehicle routes and schedules are decided simultaneously with delivery amounts and visiting times. A wide range of constraints, which include access windows of customers, maximum working/driving time limit for drivers, and vehicle capacities, make IRP a hard problem. To address this challenge, we have developed advanced solution methods, including preprocessing and decomposition methods.

First, in the preprocessing algorithm, we eliminate some nodes and arcs in the SC network that are very unlikely to be visited or used in the current horizon. Based on the information of real-time inventory levels, estimated future consumption and customer locations, the preprocessing algorithm reduces the size of the SC network by removing some redundant nodes and arcs for the current horizon.

Second, the proposed decomposition method considers an upper level vehicle routing problem, and a lower level scheduling problem. The upper level vehicle routing problem determines the optimal routes and route-vehicle pairings to minimize the transportation cost while making sure that the minimum customer "demands" are satisfied (i.e., the inventory at the end of horizon is greater than a minimum terminal level). The upper level solution gives a lower bound on the minimization objective as it is a relaxation of the original problem. Using the solution of upper level problem as input, we solve the lower level distribution scheduling problem with customers, vehicles, drivers and all constraints. The lower level solution yields an upper bound, since it is a feasible solution for the IRP. The upper and lower subproblems are linked by an iterative algorithm. When the lower level scheduling problem is infeasible, or the lower bound is strictly less than the upper bound, integer cuts are generated and added to the upper level problem. The lower level infeasibility can be due to (1) an infeasible assignments of routes to a driver, (2) access window constraints, and (3) inventory level violations. The discrepancies between the upper and lower bounds can be due to longer working times or smaller delivery amounts found by the lower level problem compared to that of the upper level problem. The iterative algorithm terminates when the gap of the upper and lower bounds is closed.

Furthermore, we show how our methods account for various practical constraints. These constraints include the modeling of time-varying consumption profiles, truck-customer compatibility, serve-first requirements for some customers, and penalization of low inventory levels. Finally, we discuss instances with different products, which lead to distribution networks of various sizes.

3:20 PM **On the Alleviation of Inventory Creep in Process Scheduling** (FrB1e)

Yazeed Aleissa, Donald J. Chmielewski (Illinois Institute of Technology)

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

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

[1]. Lima, R. M.; Grossmann, I. E.; Jiao, Y. "Long-term scheduling of a single-unit multi-product continuous process to manufacture high performance glass." Comput. Chem. Eng. 2011, 35 (3), 554−574.

[2]. Omell, B.P.; D.J. Chmielewski, "IGCC Power Plant Dispatch using Infinite-Horizon Economic Model Predictive Control" Ind. Eng. Chem. Res., 52(9) pp 3151-3164 (2013).

[3]. Mendoza-Serrano, D.I.; D. J. Chmielewski, "Smart Grid Coordination in Building HVAC Systems: Computational Efficiency of Constrained ELOC " Sci. Tech. Built Env., in press (2015)

[4]. Omell, B.P.; D.J. Chmielewski, "On the Stability of Infinite Horizon Economic MPC," Annual Meeting of the AIChE, San Francisco, CA, 2013.

[5]. Peng, J.K.; A.M. Manthanwar; D.J. Chmielewski, "On the Tuning of Predictive Controllers: The Minimally Backed-off Operating Point Selection Problem," Ind. Eng. Chem. Res., 44, pp 7814-7822, (2005).

Tissue Engineering II

Friday, March 4, 2016 (Armour Dining, **FrB2**)

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

Co-Chair: *Chenlin Lu* (Illinois Institute of Technology)

2:00 PM **Macrophage Activation and Reprogramming is Dependent on Crosslinking Density of Hyaluronan Hydrogels** (FrB2a)

Jamie E. Rayahin, Richard A. Gemeinhart (University of Illinois at Chicago)

Biomaterials used in regenerative medicine and tissue engineering interact with the surrounding microenvironment and their success is ultimately dependent on this interaction. Macrophages are highly plastic host immune cells, which persist for the lifetime of the biomaterial and have the robust ability to promote integration or rejection dependent on their polarization.

Hyaluronan (HA) has been extensively explored in regenerative medicine for its favorable mechanical properties and natural derivation. We have previously shown that as a free polymer, HA promotes molecular weight-dependent gene expression and cytokine secretion. High molecular weight HA (HMWHA) can induce an alternative activation of macrophages, regardless of the initial polarization state of the macrophage, endowing pro-wound healing, pro-resolving, and tissue regenerative qualities to the macrophage. However, although there is a widespread use of HA in cross-linked systems, there is a paucity of data on the influence of cross-linked HA on macrophage function. With this in mind, we set out answer the question: what influence does molecular weight between crosslinks have on HA's ability to modulate macrophage function? We hypothesized that as molecular weight between crosslinks decreased, HA's ability to alternatively activate a macrophage would also be reduced.

Hydrogels with differing molecular weights between crosslinks were prepared from HMWHA using various amounts of a bis-epoxide crosslinker, 1,4-butanediol diglycidyl ether. Cytokine naïve and polarized (alternative or classical) macrophages were introduced to the hydrogels. Functional responses of these macrophages to the hydrogels were determined by examining shifts in phenotype-selective mRNA, including expression of nos2, arg1, il12b, il10, cd80, mrc1, and tnf and production of nitric oxide and TNF-alpha. We found that all hydrogels maintained anti-inflammatory properties. Hydrogels with the largest molecular weight between crosslinks preserved the greatest resemblance of an alternatively activated-like state of the macrophage.

We conclude that cross-linking HMWHA to form hydrogels, although retaining anti-inflammatory properties of HMWHA polymers, diminishes the ability to robustly promote alternative activation of macrophages. HMWHA's intrinsic material properties in modulating macrophage phenotype are maintained to the greatest extent in HA hydrogels with larger molecular weights between crosslinks.

2:20 PM **Tether Strength of Cell Adhesion Ligands Modulates Biological Activities of a Cell-Laden Hydrogel** (FrB2b)

Jooyeon Park, Min Kyung Lee, Xuefeng Wang, Mehdi Roein-Peikar, Taekjip Ha, Hyujoon Kong (University of Illinois at Urbana-Champaign)

There have been many attempts to control cell behavior through material stiffness and patterning. In this study, we controlled the ultimate bond strength of the linker connecting the hydrogel and cell adhesion peptide to regulate cell adhesion, differentiation, growth factor secretion, and angiogenesis. In order to regulate the tethering strength of the linker, we utilized deoxyribonucleic acid (DNA) tethers that have different rupture forces by controlling the force application geometry. The rupture force of DNA tethers was the smallest in the unzipping geometry and highest in the shear geometry. Mesenchymal stem cells showed enhanced adhesion, differentiation, and paracrine secretion when cultured on DNA tethers with higher rupture forces, which stimulated angiogenesis in vivo. Our findings propose that the interfacial engineering of the hydrogel scaffolds by modulating the tether strength of cell adhesion epitope can play a crucial role in cell engineering.

2:40 PM **Development of Hydrogel Nanoparticles for Sustained Delivery of Angiogenic Peptides** (FrB2c)

Daniel A. Young, Marja Bittencourt, Luana Dias, Wesley Lo, Fouad Teymour, Georgia Papavasiliou (Illinois Institute of Technology)

A critical criterion for the clinical success of hydrogel scaffolds is their ability to promote rapid and stable neovascularization upon implantation prior to material degradation. Previous studies have shown that controlled and sustained growth factor presentation in hydrogels leads to enhanced and stabilized vessel formation. A promising alternative to the use of growth factors are synthetic growth factor mimetic peptide sequences designed to interact with the specific receptors growth factors use to regulate neovascularization while allowing for high ligand specificity and ease in synthesis. A peptide mimetic sequence, QK, has been previously developed and shown to activate the signaling pathway involved in vascular endothelial growth factor (VEGF)-mediated neovascularization. We have developed crosslinked hydrogel nanoparticles (NPs) of polyethylene glycol (PEG) that allow for sustained release of QK to control its delivery in scaffolds. QK loaded NPs were formed using a previously developed inverse phase miniemulsion polymerization protocol. In this study we optimized the polymerization kinetics of the NP synthesis process to allow for controlled adjustments in NP crosslink density and degradation. This was achieved through alterations in PEG crosslinker molecular weight, adjustments in PEG crosslinker concentration while maintaining the total moles of reactive double bonds constant, or by rendering the macromer hydrolytically degradable. Nanoparticle tracking analysis revealed that the average particle diameter (~236.0 nm) was unaffected by the different NP formulations. By day 21, 38.5% of entrapped peptide was released for the control case; 25.6% from NPs with high crosslink density; 49.5% from NPs with low crosslink density; and 51.2% from degradable NPs made with the same formulation as the control. Using a diffusion chamber the estimated diffusion coefficient of QK ranged from 1.35x10-6 to 1.76x10-6 cm2 s-1 for high and low crosslinked NPs, respectively. Future studies will investigate the bioactivity of QK from released NP samples in vitro.

3:00 PM **Multivalent Nanomaterial Arrays Leverage Antigen Specificity to Modulate Immune Response in Autoimmune Disease** (FrB2d)

Brittany Hartwell, Heather Shinogle, Bradley Sullivan, Laura Northrup, Cory Berkland (University of Kansas)

Introduction:

Many current therapies for autoimmune diseases such as multiple sclerosis (MS) act through nonspecific targeting of the immune response, rendering global immunosuppression, poor efficacy, and adverse side effects. To address a pressing need for safer and more effective therapies, we have developed multivalent soluble antigen arrays (SAgAs), designed to induce antigen-specific tolerance in MS. SAgAPLP:LABL consists of a flexible hyaluronic acid (HA) linear polymer cografted with multiple copies of autoantigen (proteolipid protein peptide, PLP¬139-151) and adhesion inhibitor (ICAM-1 inhibitor peptide, LABL). These peptides may enable SAgAPLP:LABL to target and interrupt antigen-specific signaling between antigen presenting cells (APCs) and T cells to halt propagation of an autoimmune attack. Previous in vivo studies showed SAgAPLP:LABL is therapeutically effective against EAE, a murine model of MS. To elucidate therapeutic cellular mechanisms, we investigated the hypothesis that SAgAPLP:LABL exhibits enhanced, antigen-specific binding with APCs and modulates signaling.

In vitro studies were performed in a model B cell system using flow cytometry to evaluate binding and specificity. SAgAPLP:LABL exhibited greatly enhanced binding compared to HA and HA arrays containing only PLP or LABL. Furthermore, specific binding was primarily driven by the PLP antigen, determined by flow cytometry competitive dissociation studies. Fluorescence microscopy, performed in real-time utilizing a microfluidics platform, showed that SAgAPLP:LABL induced mature receptor clustering in B cells to a greater extent than other HA arrays. SAgAPLP:LABL also reduced and inhibited IgM-stimulated signaling, as discerned by a flow cytometric calcium flux assay. Lastly, SAgAPLP:LABL exhibited greater binding ex vivo in murine EAE splenocytes over healthy splenocytes. Leveraging enhanced, antigen-specific binding and signaling modulation, SAgAPLP:LABL offers a promising option for antigen-specific immunotherapy to repress autoimmune disease.

3:20 PM **Modular Crosslinking of Gelatin Based Thiol-Norbornene Hydrogels for In-Vitro 3D Culture of Hepatocellular Carcinoma Cells** (FrB2e)

Tanja Greene, Chien-Chi Lin (Purdue University)

Gelatin-based hydrogels are increasingly used to promote cell fate processes in 3D. Here, we report the use of orthogonal thiol-norbornene photochemistry to prepare modularly crosslinked gelatin-based hydrogels for the in vitro studying of the influence of independent matrix properties on hepatocellular carcinoma cell fate in 3D. In addition to demonstrating the ability to independently tune the mechanical and biological properties of modular gelatin-norbornene (GelNB) hydrogels, we also determined that network crosslinking density plays a key role in the mechanisms of proteolytic gel degradation. During in vitro degradation studies, GelNB hydrogels with lower crosslinking density degraded faster and followed a surface erosion mechanism, whereas dense GelNB hydrogels degraded in a bulk degradation mechanism. Hepatocellular carcinoma cells, Huh7, were encapsulated and grown in GelNB hydrogels with modularly tuned stiffness, bioactive motifs, and heparin content to systematically evaluate the effect of matrix properties on cell viability and functions, including CYP3A4 activity and urea secretion. We found that encapsulated Huh7 cells exhibited higher cellular metabolic activity when encapsulated in modular GelNB hydrogels composed of higher gelatin contents or gels with lower stiffness. Interestingly, altering gelatin content and matrix stiffness did not significantly affect hepatocyte-specific cellular functions. To improve cellular function, we prepared norbornene and heparin dual-functionalized gelatin through a two-step synthesis protocol. Heparin-functionalized GelNB (i.e., GelNB-Hep) hydrogels were able to sequester and slowly release hepatocyte growth factor (HGF). Finally, the conjugation of heparin on GelNB led to suppressed Huh7 cell metabolic activity and improved hepatocellular functions.

Refining and Petrochemical Engineering II

Friday, March 4, 2016 (Alumni Lounge, **FrB3**)

Chair: *Victor Sussman* (Dow Chemical Company)

Co-Chair: *Juan Salazar* (UOP/Honeywell)

2:00 PM **Reactor Internals for Hydroprocessing Units** (FrB3a)

Henrik Rasmussen (Haldor Topsoe, Inc.)

The catalyst companies are continuously developing more active catalyst to meet more stringent product specifications. In order to fully utilize today's catalyst technology it is imperative that the hardware is upgraded as well. Many of today's hydroprocessing units are using reactor internals designed 30+ years ago. Furthermore the feeds are different and the feed rate is most likely higher compared to the initial design, making it necessary to utilize new and properly designed, distribution trays, mixing chambers and scale catchers. The presentation will also highlight how improved safety for the people working with the trays have been included in today's optimized design.

2:40 PM **Hydroprocessing Revamps for Maximum Flexibility and Profitability** (FrB3c)

Sudhakar Chakka, Laura Kadlec (UOP)

Refiners are facing unique challenges in today's competitive and unstable markets to stay profitable. Some of the ways refiners are trying to increase their feed and product flexibility and therefore profitability, are:

- More efficient utilization of the existing assets,

- Processing increasing proportion of cheaper opportunity crudes including Tight Light Oils (Shale) and Heavy Crudes, and
- Increasing the yields of desirable products while lowering the yields of undesirable products, and producing higher value products such as Lubes.

However, refiners are finding that they need help in implementing these profit-enhancing improvements in their aging process units that are designed for easier feed and less stringent product specifications. Continuously increasing mandated fuel quality specifications are only making this effort more difficult.

With 100 years of stellar history, continuous innovation and experience, UOP offers a variety of revamp engineering services and process solutions to meet refiners' needs. UOP is uniquely qualified to perform revamp engineering because UOP has the process and catalyst knowledge to alter key process parameters and/or process flow schemes for the most effective utilization of the existing equipment to meet desired objectives. UOP can also recommend any new process equipment and/or equipment revamps where appropriate to help refiners to meet their stretch goals and achieve trouble free operation.

Topics to be presented include:

- UOP's unique Catalyst, Process, and Engineering solutions for increasing throughput, increasing the yields of desirable products, and increasing conversion in hydrocrackers to 99+%, running opportunity crudes, energy saving solutions, and achieving flexibility to switch between gasoline and diesel production in hydroprocessing units.
- UOP's latest engineering innovations that improve efficiency and reliability, and for debottlenecking Hydroprocessing units.

3:00 PM **Maximizing Reliability and Profitability in Hydrogen Plant Designs** (FrB3d)

Diane Dierking (Johnson Matthey Process Technologies)

Tightening fuel specifications, increase in hydrocracking capacity and the upgrade of the hydrogen deficient bottom of the barrel mean that most refineries will be investing in on-purpose hydrogen production, if they have not already. As this trend is likely to continue unabated for at least the next two decades (Hart), this paper critically reviews trends in the design of modern hydrogen plants and examines how they can best be integrated into refinery operations.

The hydrogen plant flow sheet has not altered much in the last 20 years following the adoption of PSA separation technology. Small, older-generation hydrogen plants used to operate much as a utility, providing top-up supply to the refinery hydrogen balance. Today these are being replaced with much larger units (some exceeding 200 MMSCFD), and many of which are being run close to design capacity. With these newer units, on-stream reliability is crucial to refinery profitability. The paper explains why newly constructed hydrogen plants have so far mainly been designed as larger versions of their older cousins, and contains suggestions for changing this trend.

There are many areas that the refiner needs to consider when defining the scope for a new hydrogen plant. These include:

- Feedstock flexibility: Feedstock flexibility offers the refiner more choice in selecting cost effective feeds. However, this has to be balanced against a higher initial capital cost, shorter operating lives of some catalysts and in some cases a less robust or reliable plant.
- Steam export: Export steam can be a valuable byproduct to the refiner. There are, however, ways to minimize export steam if the value is low or alternate uses that could be considered, such as power generation or to drive compressors.
- Feed specifications: Oftentimes feed specifications are inconsistent with known information. This paper will explain the common pitfalls and show how these can be simplified to produce a more cost-effective and efficient plant design.
- Catalytic: Hydrogen plants use several different catalyst and absorbent technologies, with volumes often increased during the design phase to allow the use of products from various catalyst suppliers. However, limiting supplier choice simply can reduce the cost of the plant.
- Capital cost reduction: The paper provides several examples where simple cost trimming at the design phase has resulted in long-term problematic hydrogen plant operation, and provides recommendations for avoiding such pitfalls.

It is important that these decisions are well thought through by the refiner before approaching technology vendors to design the plant. This ensures that the refiner gets more value for their investment – a reliable process that does exactly what it was intended to do, in a cost effective manner.

Hydrogen production is no longer a simple utility operation. It is key to the reliable operation of today's complex refineries. This paper draws on years of experience in the design and operation of hydrogen plants to help guide the refiner when making such large and strategically important investment decisions.

3:20 PM **Methanol to Olefins (MTO) - Market and Technology Review** (FrB3e)

Joseph Montalbano (UOP)

The Methanol to Olefins (MTO) process has been an increasingly important means to produce ethylene and propylene. This presentation will identify the market for ethylene/propylene technologies and will review MTO process technology.

<u>Pharmaceutical Processing</u>

Friday, March 4, 2016 (Herman Lounge, **FrB4**)

Chair: *Hamid Arastoopour* (Illinois Institute of Technology)

Co-Chair: *Vahid Mirshafiee* (University of Illinois at Urbana-Champaign)

2:00 PM **Optimization of Batch and Continuous Cooling Crystallization of High Aspect Ratio Crystals under Nucleation, Growth, Dissolution and Breakage for Shape Control** (FrB4a)

David Acevedo, Zoltan K. Nagy (Purdue University), *Christopher L. Burcham, Daniel J. Jarmer* (Eli Lilly & Co.)

Batch and continuous cooling crystallization of potassium dihydrogen phosphate in an impure media is evaluated through the implementation of various optimization frameworks to assess the achievable crystal size and shape. The continuous system studied is a two-stage mixed-suspension mixed-product removal (MSMPR) crystallization process. The systems are modelled using a multi-dimensional population balance model under nucleation, growth, and dissolution kinetics. The impact of agitation rate is studied by considering a binary crystal breakage model. A significant decrease in the achievable aspect ratio is observed by controlling the dissolution of crystals (batch scenario) and limiting the residence time and growth (continuous scenario). Further improvement of the final shape is achieved by considering the agitation rate in the optimization framework. However, the increase in the variance of the crystal mean size and aspect ratio indicates a trade-off between the aspect ratio and spread of the crystal size distribution. Nonetheless, this work illustrates promising results for further development of process optimization frameworks and control approaches for batch or continuous cooling crystallization operations by considering multiple crystallization kinetics and binary crystal breakage kernels, which can be used as a generic model-based design framework for batch and continuous crystallization processes of needle shaped particles to achieve desired mean aspect ratio.

2:20 PM **Analyzing the Effect of Material Properties on a Twin Screw Wet Granulation Process** (FrB4b)

Shankali Pradhan, Maitraye Sen, Carl Wassgren, James Litster (Purdue University), *Ian Gabbott, Gavin Reynolds* (AstraZeneca)

Wet granulation is an important unit operation often implemented by solid handling industries (Pharmaceutical, Chemical, Food etc.) for size enlargement of fine powder particles to improve handling and downstream processing of particulate solid material. The properties of the product (granules) obtained from a wet granulation operation is sensitive to the equipment design, different process parameters and material properties of the primary powder. The effects of different process parameters and material properties have been studied extensively for high shear mixer granulators in literature [1]. In pharmaceutical industries, with the onset of continuous processing framework, a detailed study of the different continuous granulator designs is required. Continuous twin Screw wet granulation has been gaining increasing importance in the recent years because of its short residence time, small equipment footprint and flexible and sequential design [2]. The objective of the present work is to study the effect of material properties of the primary powder on the granule characteristics obtained from a twin screw granulator (TSG). The material properties which have been considered are dynamic yield strength, drop penetration time and shear properties of the primary powder. Different model materials have been chosen which give variation in the above mentioned material properties and their effect on the granulation rate processes in a TSG have been studied. Studies have been carried out using different pharmaceutical formulations (multi-component systems) as well. A critical evaluation of these results will be presented and the impact of material properties on granule attributes will be compared.

[1]. Reynolds et al., 2005. Chemical Engineering Science, 60, 3969-3992

[2]. Sayin et al., 2015. International Journal of Pharmaceutics, In press,doi:10.1016/j.ijpharm.2015.09.024

Acknowledgement: The authors acknowledge the assistance of Jiayu Li in conducting the experiments.

2:40 PM **Estimation of the Breakage and Selection Function in the Roller Compaction Process** (FrB4c)

Mariana Moreno, Sudarshan Ganesh, Gintaras V. Reklatis, Zoltan K. Nagy, Alexander R. Milaszewski, Isaac E. Mendoza (Purdue University)

The roller compaction process is a dry granulation method and it is widely-used in the pharmaceutical manufacturing [1]. Modeling this process give us a better process understanding and, as a consequence, potential improvements on the quality of the product. The parameters used in the roller compactor can impact the quality of the product since they have an effect on the granules particle size distribution (PSD). For instance, the bulk density of the roller compacted ribbon can change the PSD of the granules [2].

In order to represent the milling unit operation, a population balance is needed. Therefore, estimating the parameters for the breakage and selection function of the mill is required [3]. These parameters are estimated by varying the mill speed, the composition of the material and the density of the ribbon. The particle size distribution is measured online and offline. At the end, a comparison of the estimated parameters is made.

[1]. Miller, R.W.; Sheskey, P. J. Roller Compaction Technology for Pharmaceutical Industry. 2003. Marcel Dekker Inc. New York, New York.

[2]. Yu S. Roll Compaction of Pharmaceutical Excipients. 2012, The University Birmingham, UK.

[3]. Pettersen J. & Sandvik K. Estimating the breakage and selection function for a continuous mill. International Journal of Mineral Processing. 1992, 35, 149-158.

3:00 PM **Development of Drug Nanocrystals for Intravenous Injection** (FrB4d)

Tonglei Li (Purdue University)

Chemotherapy is widely used to treat cancer. It is nonetheless accompanied by terrible side-effects resulting from the ubiquitous exposure in the body to cytotoxic chemicals that are intended to eliminate malignant cells. Compounding the systemic toxicities is the universal utilization of carrier chemicals to deliver the chemotherapeutic drugs. The carrier chemicals, which solubilize and/or encapsulate drug substances into various dosage forms, lead to possibly detrimental effects and likely contribute to the problems of overtreatment. For this, we have developed carrier-free drug nanocrystals for chemotherapy over the last few years. The platform aims to deliver nanosized crystalline particles without using any solubilizing or encapsulating chemicals. The nanocrystals may be administered directly through intravenous injection. Our in vitro and in vivo studies demonstrate that not only the treatment efficacy is comparable and better than the conventional treatments, but the toxic reactions are significantly reduced, largely due to the absence of carrier chemicals. Furthermore, by surface-coating biocompatible polymers onto drug nanocrystals, additional improvement on biodistribution and toxic side effects have been observed. Pharmacokinetic modeling and simulation studies have been undertaken to understand the impact by particle properties, including surface chemistry and particle size, on the biodistribution and pharmacodynamics.

3:20 PM **Application of Automated Direct Nucleation Control in Continuous Cooling Crystallization and Wet Milling Processes** (FrB4e)
Yang Yang, Liangcheng Song, Zoltan K. Nagy (Purdue University)

Continuous crystallization is of great interest in pharmaceutical and fine chemical industries due to its enhanced product quality consistency, improved process and equipment efficiency, and reduced operation cost compared to batch crystallization. Therefore the development of automated and robust control of continuous crystallization process is extremely important.

A fully automated focused beam reflectance measurement (FBRM) based closed-loop control approach, which is named as automated direct nucleation control (ADNC), is proposed and implemented to control particle size distribution (PSD) in continuous cooling crystallization and wet milling processes. FBRM is an extensively used process analytical technology (PAT) that provides in situ particle chord length distributions, which can be related to the number and size of the particles present in the system. This information is used in the proposed ADNC approach to automatically adjust the jacket temperatures of the crystallizer and the wet mill.

The proposed ADNC approach is successfully implemented and evaluated in three continuous crystallization and wet milling processes: (1) Continuous mixed suspension mixed product removal crystallizer (MSMPRC) without wet mill; (2) Continuous MSMPRC with rotor-stator wet mill operated upstream for continuous in situ seed generation; (3) Continuous MSMPRC followed by rotor-stator wet mill operated downstream through recycling for continuous size reduction. The proposed ADNC approach is observed to provide quick startup, high quality control of PSD, and effective disturbance rejection.

(Canceled) **Process Safety Workshop I**
~~Friday, March 4, 2016 (Crown Room, **FrB5**)~~
Chair: Brenton L. Cox (Exponent Inc.)
Co-Chair: Peter Hereña (Baker Engineering and Risk Consultants, Inc.)

(Canceled) 2:00 PM **Process Hazards Analysis** (FrB5a)
Peter Hereña (Baker Engineering and Risk Consultants, Inc.)

A Process Hazards Analysis (PHA) is a required activity for operating companies that must comply with OSHA 29 CFR 1910.119, the regulation that governs Process Safety Management (PSM). It is a good practice for any company, regardless of applicability of the PSM regulation, to understand and manage process safety hazards in a chemical processing environment. The concept has been successfully applied to many types of systems beyond the industrial manufacture of chemical products.

A PHA can consist of many different techniques, from the simple “What-If?” analysis, to the commonly applied Hazard and Operability Analysis (HAZOP), extending to sophisticated and detailed modeling of a Quantitative Risk Analysis (QRA). Besides the methods mentioned above, there are many more that reside under the umbrella of good PHA methods. This workshop will discuss the different methodologies, their advantages and disadvantages, and will promote discussion on factors to consider when deciding which method to choose for your application.

(Canceled) 2:55 PM **Safe Work Practices** (FrB5b)
Brenton Cox, Sean Dee (Exponent Inc.)

Hot work, lockout/tagout, and confined space entry are examples of non-routine work activities where existing engineering and administrative controls may be bypassed, disabled, or replaced with temporary safeguards to facilitate work activity. In these scenarios, the risk of experiencing a process safety incident is heightened unless the hazards are otherwise effectively managed. Safe work practices including job safety analyses, work permits, and checklists are additional control measures employed to manage this risk.

This session will review a series of case studies involving process safety incidents that occurred during non-routine work activities, highlighting the hazards associated with these activities, along with issues related to regulatory compliance. We will also summarize guidance from various sources aimed at improving hazard mitigation, worker safety, and regulatory compliance.

Leadership Workshop

Friday, March 4, 2016 (Armour Conference Room, **FrB6**)
Chair: *Alfred Nunez* (Illinois Institute of Technology)

2:00 PM **Interactive Workshop on Leadership Excellence** (FrB6a)
Manu Vora (Business Excellence Inc.)

In this interactive workshop we will discuss leadership excellence. You will learn various leadership characteristics. Difference between a leader and manager will be explored. You will examine your own leadership characteristics. Excellent leadership models will be discussed. We will sketch out a roadmap for leadership excellence and development. You will learn key concepts, best practices, and practical tools to enhance your leadership excellence.

Sustainable Power Systems

Friday, March 4, 2016 (Ballroom, **FrC1**)
Chair: *Dennis O'Brien* (Jacobs Consultancy)
Co-Chair: *Yazeed Aleissa* (Illinois Institute of Technology)

4:00 PM **Numerical Modeling of CO_2 Desorption Process in a Carbon Capture Unit using the Fluidized Bed Process** (FrC1a)
Emad Ghadirian, Hamid Arastoopour, Javad Abbasian (Illinois Institute of Technology)

One of the promising approaches to Carbon Capture and Storage (CCS) is to use solid sorbents and fluidized bed process, although this process currently is not ready for implementation in industrial scale plants. One of the major challenges is the fact that it is still in the lab or bench scale stages. To successfully scale-up such processes, a powerful tool, i.e. Computational Fluid Dynamics (CFD), is needed. In order to have steady CO2 capture using solid sorbents, a circulating fluidized bed (CFB) is used which consists mainly of a carbonator reactor (where the CO2 is adsorbed by solid sorbents) and a regenerator (where carbonated sorbents release CO2 and a concentrated CO2-steam mixture is produced). Different solid sorbents have been developed to be utilized in carbon capture units such as MgO-based sorbets and CaO-based sorbents. In this study, MgO-based solid sorbent was used due to its capability to capture CO2 at high temperature (300-550 °C) which is in the vicinity of the operating conditions of advanced power plants (e.g. integrated gasification combined cycles [IGCC]). This results in a lower energy penalty in the carbonation/regeneration cycle of MgO-based sorbents. In this study three dimensional CFD simulations of the regeneration unit of carbon capture process using MgO-based solid sorbents were investigated and performance of the fluidized bed regenerator unit, operating at different conditions, was studied. An Energy Minimization Multi Scale (EMMS) approach was used to calculate the drag force between gas and solid phases in Eulerian-Granular (also known as two fluid model [TFM]) approach and a Shrinking Core model was utilized to model the heterogeneous regeneration reaction.

4:20 PM **High-Gravity Carbonation Process for Carbon Capture and Utilization Exemplified by Steelmaking Industry** (FrC1b)
Shu-Yuan Pan, Silu Pei, Pen-Chi Chiang (National Taiwan University), *Yupo J. Lin* (Argonne National Laboratory), *Yi-Hung Chen* (National Taipei University of Technology)

In this study, a high-gravity carbonation (HiGCarb) process using rotating packed bed for CO2 capture, wastewater neutralization and product utilization was developed and deployed in steelmaking industry. A high CO2 removal ratio, i.e., >98%, was achieved by utilizing basic oxygen furnace slag and cold-rolling wastewater via the HiGCarb process with a relatively short reaction time at ambient temperature and pressure. The objectives of this study were (1) to evaluate the resource potential of alkaline solid wastes in Taiwan for CO2 capture and utilization using the HiGCarb process in Taiwan, (2) to quantify the pollution emissions and environmental impacts of the HiGCarb process from the cradle-to-gate life-cycle, (3) to calculate the water, carbon, and land footprints of the HiGCarb process, and (4) to establish the cost and benefit analysis of the HiGCarb process at an industrial-plant scale. The alkaline wastes were found to be successfully carbonated with CO2 in the HiGCarb process, where calcite (CaCO3) was identified as the main product. Since the reacted product (e.g., carbonated solid wastes) can be used as supplementary cementitious materials, CO2 emissions from the cement industry can be also avoided if a green waste-to-resource supply chain between the steelmaking and cement industries is established. It was concluded that an integrated approach to the proper treatment of alkaline wastes that permanently fixes CO2 from the petrochemical industry while producing valuable supplementary cementitious materials for the cement industry can be achieved via the HiGCarb process.

4:40 PM **Exploiting Electricity Markets for Better Systems Engineering** (FrC1c)
Alexander Dowling, Victor Zavala (University of Wisconsin Madison)

Awareness of variable electricity prices is ubiquitous in recent systems engineering literature, with board applications including planning and scheduling for flexible manufacturing facilities, renewable energy system design, evaluation of new energy storage technologies, and intelligent building operations. In most energy markets, however, multiple energy "products" are sold on different timescales, with spatial variations in prices. As consequence, using simplistic "off-peak" and "on-peak" pricing structures may not be sufficiently accurate in many geographic regions. Thus a deep understand of electricity markets organization and the associated hierarchical control is required to accurately model price signals.

In this talk, we will review electricity markets in the United States, with an emphasis in the following areas:

- Timescales of variations in electricity demand and prices

- Basic regulatory agencies and structure in the United States
- Market-based control hierarchy for the California electricity grid
- Role of ancillary services and associated revenue opportunities
- Review of market-based economic analysis literature for energy storage system

The aim of this talk is to provide the necessary background for audience members to read market specific rules and analyze historical data (which is available online to the public for many US markets).

5:00 PM **On the Use of Multistage Stochastic Programming for the Design of Grid Scale Energy Storage Systems** (FrC1d)
Oluwasanmi Adeodu, Donald J. 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.

Due to the uncertainty of consumer demand as well as that of renewable generation, the problem of optimal placement of these storage units within the grid along with the selection of equipment sizes must be formulated as a stochastic program. However, rather than being a fairly simple two-stage stochastic program, the dynamics imposed by the storage devices requires the formulation to be of the far more challenging multistage class.

In this work, we propose a novel approximate solution procedure for this class of multistage stochastic programming problems. The approach utilizes the computational efficiency of the recently developed method of Economic Linear Optimal Control (ELOC) and its extension Constrained ELOC. The proposed method occurs in two stages. The first is a global search over the here-and-now variables as well as the parameters of the ELOC policy. However, this first search assumes a statistical constraint enforcement mechanism (similar to chance constrained optimization). In the second step is a gradient based search over the here-and-now variables, but used the Constrained ELOC policy to enforce point-wise-in-time constraints. To address the possible occurrence of an infeasible solution from the Constrained ELOC policy a fairly simple barrier type approach is used to improve convergence properties.

5:20 PM **Optimal Design and Control of CCHP Systems for Housing Complexes** (FrC1e)
Luis Fabián Fuentes Cortés (Universidad Michoacana de San Nicolás de Hidalgo), *Alexander Dowling, Victor M. Zavala Tejeda, José Maria Ponce Ortega* (University of Wisconsin Madison)

In the residential sector of Mexico, the most important energy demands are related to the supply of electricity, cooling and sanitary hot water. These demands can be met efficiently using trigeneration systems (Combined Cooling Heat and Power, CCHP). However, the design of CCHP systems involves three interrelated layers of decisions: technology selection, equipment sizing and operation policies of the central CHP unit and water storage. We formulate this design problem as a multi-objective stochastic mixed-integer nonlinear program (MINLP). The optimization problem includes internal combustion engine, fuel cell, microturbine, Stirling engine, water heaters and absorption chiller technology options, and considers the sizing equipment such as the hot storage tank(s). Optimal operating policies are considered using daily scenarios based on real data for ambient temperature, fuel costs, electricity prices and user demands. This approach is preferred over using seasonal historical averages, which may lead to undersized equipment with respect to extreme circumstances (e.g., an abnormal week of weather). Finally, Pareto optimal trade-offs between total annual operating costs and greenhouse gas emissions are developed using the ε-constraint technique. The methodology is demonstrated for a housing complex of 420 households located on the Pacific Coast of Mexico.

<u>Modeling of Biological Systems</u>

Friday, March 4, 2016 (Armour Dining, **FrC2**)
Chair: *Seok Hoon Hong* (Illinois Institute of Technology)
Co-Chair: *Daniel Young* (Illinois Institute of Technology)

4:00 PM **Spatio-Temporal Engineering of Biochemical Reaction Networks** (FrC2a)
Milan Mrksich (Northwestern University)

The reactions of molecules in the cell occur in highly non-uniform settings. Enzymes, cofactors, and substrates are rarely present at uniform concentrations throughout the cell but rather are spatially organized into regions of high and low concentration. These concentration profiles and the ways in which they are temporally regulated are essential to the normal operation of the reaction networks that underlie cell function. Yet, mechanistic studies of the unique factors that stem from spatio-temporal structuring of reactants are challenging. This seminar will describe a model system wherein enzymes act on immobilized substrates, with several unusual features. We show that a kinase which can associate with the phosphopeptide it generates will display an autocatalytic reaction profile. Further, the reaction generates spatial patterns of the product and shows an initial rate that varies with geometrical pattern, but not the ratio, of substrate and product. When reactions are performed in the presence of an opposing phosphatase, the direction of the phosphorylation reaction shows a dependence on the density of the substrate. This last observation points to a new motif for regulating phosphorylation events at the cell membrane and we engineer cells that display a kinase-dependent transmembrane signaling event in response to clustering of a chimeric receptor. This work provides an example of the unique features that derive from biochemical reactions in non-uniform environments.

4:20 PM **High Definition (HD) Fourier Transform Infrared (FT-IR) Spectroscopic Imaging for Rapid Chemical Analysis** (FrC2b)

Shachi Mittal, Rohit Bhargava (University of Illinois at Urbana-Champaign)

The molecular-microscopic chemical underpinnings of materials, from polymer composites to human tissue, determine their function. HD FT-IR spectroscopic imaging is a powerful emerging tool to provide molecular fingerprints of samples in an imaging format, non-invasively and without the need for additional contrast agents or dyes. It can greatly expedite the process of identification of complex molecular constituents by the use of automated and efficient pattern recognition tools. These tools combined with the inherent biochemical understanding of the sample will be utilized to identify the most relevant spectral attributes for classification. In the example application here, we show how this emerging technology can be used to augment current practice in cancer diagnosis. Further, we optimize the developed protocols by targeting collection of discrete frequencies, significantly accelerating the IR imaging. Finally, we optimize our model systems for different levels of noise in the recorded data, illustrating opportunities for control. These integrative approaches will make disease diagnosis using HD FT-IR imaging more robust, time efficient and less expensive.

4:40 PM **Modeling and Prediction of Antibody Production in Mammalian Cell Culture - Dual Rate Approach** (FrC2c)

Jingwei Gan, Satish J. Parulekar, Ali Cinar (Illinois Institute of Technology)

Multirate systems, where inputs and/or outputs have different sampling rates, are encountered in many engineering applications such as digital signal processing and process control and estimation. Typically, this occurs in systems where multiple variables are measured. Process variables such as temperature, pressure and pH are measured more frequently, at times nearly continuously, while other variables, such as species concentrations in a reaction mixture, are measured less frequently. An example of such processes is mammalian cell culture, where sampling rates for viable hybridoma cells, carbon and nitrogen sources, lactate, ammonia, and monoclonal antibody are significantly different.

The simplest way to handle multi-rate systems is to neglect excess data from fast sampling signals and synchronize the signals with the slowest sampling rate. With this method, great amount of data will be discarded, the data that may contain crucial information regarding system dynamics. Therefore, many efforts have been devoted to analyze and solve multi-rate systems to take advantage of the rich information available. Among all the technique proposed, multi-rate systems are generally simplified to multiple dual rate systems where the slower sampling rate is a positive integer (q) multiple of the faster sampling rate. One of the most successful techniques, polynomial transformation technique, can successfully transfer single rate models into dual rate models with ease. The dual rate model, after transformation, can utilize dual rate signals simultaneously. For such model structures, multiple identification techniques have been proposed with good estimation accuracy and convergence rate. In this work, a second order discrete time system is considered to show converge of proposed parameter estimation algorithm for dual rate model. Converge rate and estimation accuracy for multiple q is listed to comment on the existing dual rate parameter estimation technique. Use of a dual rate model with parameter estimation technique for modeling and prediction of mammalian cell culture is proposed here. The faster sampling rate corresponds to viable hybridoma cell concentration and the slower sampling rate corresponds to glucose and glutamine concentrations. The performance of the dual rate model with frequent parameter estimation in prediction of mammalian cell culture producing monoclonal antibody is examined in considerable detail.

[1]. Raghavan, H. et al., "Identification of chemical processes with irregular output sampling." Control Engineering Practice 14.5 (2006): 467-480.

[2]. Ding, J. and F. Ding, "The residual based extended least squares identification method for dual-rate systems." Computers & Mathematics with Applications 56.6 (2008): 1479-1487.

[3]. Ding, J. et al., "A modified stochastic gradient based parameter estimation algorithm for dual-rate sampled-data systems." Digital Signal Processing 20.4 (2010): 1238-1247.

5:00 PM **A Cell-Free Framework for Rapid Biosynthetic Pathway Prototyping and Enzyme Discovery** (FrC2d)

Ashty Karim, Michael Jewett (Northwestern University)

Speeding up design-build-test (DBT) cycles is a fundamental challenge facing biochemical engineering. To address this challenge, we report a new cell-free protein synthesis driven metabolic engineering (CFPS-ME) framework for rapid biosynthetic pathway prototyping. In our framework, cell-free cocktails for synthesizing target small molecules are assembled in a mix-and-match fashion from crude cell lysates either containing selectively enriched pathway enzymes from heterologous overexpression or directly producing pathway enzymes in lysates by CFPS. We apply our approach to n-butanol biosynthesis showing that Escherichia coli lysates support a highly active 17-step CoA-dependent n-butanol pathway in vitro. The high degree of flexibility in the cell-free environment allows us to manipulate physiochemical conditions, access enzymatic nodes, discover new enzymes, and rapidly prototype enzyme sets with linear DNA templates to study pathway performance. CFPS-ME facilitates a generalized approach to define, manipulate, and understand metabolic pathways for rapid DBT cycles without the need to reengineer organisms.

5:20 PM **Development of a Dynamic Cell-Free Model of B. Subtilis Metabolism** (FrC2e)
Michael Vikhovoy, Jeffrey Varner (Purdue University)
Cell-free protein synthesis (CFPS) systems are derived from crude cell extracts that contain the cellular machinery required for transcription, translation and energy metabolism. CFPS systems allow for precise control of the chemical environment without the complications associated with cell growth, genetic regulation or the cell wall. Most prokaryotic CFPS systems are E. coli based, however E. coli contains endotoxins that complicate purification. The gram-positive soil bacterium Bacillus subtilis produces 60% of commercial industrial enzymes worldwide, thus it is an ideal platform for protein production. While CFPS systems are easier to monitor and manipulate compared to in vivo systems, model based design of CFPS is lacking. We developed a dynamic cell-free model of B. subtilis metabolism by first creating an ensemble (n=1000) of whole-cell B. subtilis central carbon metabolism that includes allosteric regulation. The model was able to capture growth, glucose consumption, acetate and riboflavin production with satisfactory fits. We simulated cell-free dynamics including allosteric regulation using the same ensemble of parameter sets as the whole-cell model but removing growth-associated reactions. The cell-free system showed faster glucose consumption and higher yields of both acetate and riboflavin. This is expected, as glucose was not utilized for cell growth. The cell-free model showed transport of oxygen into the system controlled the rate of glucose consumption, which may be a key parameter for controlling CFPS systems.

<u>**CFD Methods and Applications**</u>
Friday, March 4, 2016 (Alumni Lounge, **FrC3**)
Chair: *Hadjira Iddir* (UOP/Honeywell)
Co-Chair: *Raj Venuturumilli* (BP)

4:00 PM **Computational Fluid Dynamics (CFD) for Equipment Design and Development** (FrC3a)
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.

4:20 PM **Four Phase Flow Model for Methane Production from an Unconsolidated Gas Hydrate Reservoir** (FrC3b)
Deniz Hinz, Hamid Arastoopour (Illinois Institute of Technology)
US production of natural gas from hydrate resources has the potential to provide long-term energy security, revolutionize economic growth, and improve environmental quality. To fully grasp the incredible potential of hydrates, one can compare the estimated 7000 tcf of recoverable natural gas from U.S. resource-grade hydrate deposits to the 570 tcf of technically recoverable shale gas resources which have provided the U.S. considerable economic stimulus, affordable means of decreasing coal consumption, and eliminated dependence on foreign energy resources.
Production of natural gas from hydrate resources has been deemed technically viable; however considerable questions remain regarding the complicated physics, economic feasibility and geomechanical safety over the wide range of hydrate reservoir properties. Modelling and numerical simulation provide flexible, cost-efficient means of analysis; however many aspects of the multiphase flow characteristics during hydrate dissociation are poorly understood and remain uncaptured in simulations. In particular, studies have shown that solid sand and hydrate are able to flow like unconsolidated sediment as hydrate dissociates due to loss of strength and liquefaction.
A novel mathematical model capable of predicting gas, water, and sand from unconsolidated hydrate reservoirs was developed. The initial numerical simulations have been performed for unconsolidated hydrate reservoirs using a mixture momentum model assumption and is compared with

available gas production data from the Mallik 2007/2008 production test.

4:40 PM **Computational Fluid Dynamics for FCC: Opportunities and Challenges** (FrC3c)
Raj Venuturumilli (BP)
An overview of current status of CFD usages in FCC problems will be presented to provide an assessment of where CFD may, or may not, be a helpful tool for developing the needed understanding for design and analysis of FCC units. The conclusion is that there is substantial hope that CFD could be very useful in this application but there are still multiple challenges in CFD to effectively and efficiently capture granular multiphase flow dynamics and kinetics involved in FCC.

5:00 PM **Liquid Maldistribution Study of Rocking FLNG Columns using Computational Fluid Dynamics** (FrC3d)
Pengfei Chen (UOP/Honeywell)
Offshore liquefaction of natural gas is expected to be the next technological breakthrough for capitalizing stranded natural gas resources. To access the viability and feasibility of the said FLNG (Floating Liquefied Natural Gas), marinization study is needed to evaluate and minimize the impact of sea motion on its performance. Such an impact is caused by gas/liquid maldistribution within the column with the liquid preferentially moving towards one side of the column, leaving the other side of the column depleted of the liquid. Therefore, the region with the surplus of the liquid will encounter less gas flow. The non-uniform distribution between the liquid and gas over the cross section of the column leads to the performance drop or decrease of the column efficiency. Here Computational Fluid Dynamics (CFD) is used to investigate this liquid maldistribution under different sea motion conditions.

5:20 PM **CFD Fluidized Bed Reactor Design 1. For Diesel from Shale Gas 2. For Silicon for Solar Cells** (FrC3e)
Dimitri Gidaspow (Illinois Institute of Technology)
In our recent paper (Chem. Eng. Science 134,784-799, 2015) we have shown how to use multiphase computational fluid dynamics (CFD) to design novel slurry bubble column reactors for production of Diesel fuel from natural gas produced by fracking.
This method uses the principles of conservation of mass, momentum and energy for each phase, as discussed in the text by D.Gidaspow and V. Jiradilok, Computational Techniques, Nova Science, 2009. The traditional method uses empirical hold-up correlations, as will be reviewed at the 2015 Salt Lake Annual AIChE meeting.
The first step in the production of liquids from natural gas by fracking is the formation of synthesis gas by an endothermic reaction of steam with methane. The commercial process is carried out in packed bed reactors with the heat supplied by burning extra methane. Spath and Dayton (NREL/TP 510-34929, 2003) and others have shown that such reactors account for more than 50% of the cost of producing liquids from gas. Fluidized bed reactors promise a substantial reduction in the cost of production of synthesis gas. For example, we had obtained a CFD design involving injection of oxygen into a fluidized bed. Other designs are in progress to make use of new active catalysts that promise to reduce the size of such reactors by orders of magnitude.
The majority of polysilicon is produced by the Siemens hot bar method using purified silane or trichlorosilane as the source of silicon [1]. The fluidized bed reactors offer considerably higher production rates at a smaller energy consumption leading to expected order of magnitude lower costs for solar collectors. Hsu, G. et al [2] have described the production of polysilicon from silane in a 15 cm diameter fluidized bed reactor. Their reactors, like the commercial reactors being built, are externally heated. In contrast, the proposed technique simply involves inserting electrodes, made of or coated with silicon, into the fluidized beds, connected to a high voltage supply of alternating or direct current. The voltage needed depends on the size of the reactor given by a simple expression in terms of bed resistance and required power.

[1]. Woditsch, P. and W. Koch (2002) Solar Materials and Solar Cells 72, 11-26; Ege, P.et al (2007) Intern. Patent Application Number PCT/US2006/028112.
[2]. Hsu, G. et al (1987) AIChE Journal 33, 784-791.

Environmentally Conscious Process Design
Friday, March 4, 2016 (Herman Lounge, **FrC4**)
Chair: *Pahola Thathiana Benavides* (Argonne National Laboratory)
Co-Chair: *Daniel Bampoh* (Purdue University)

4:00 PM **Lessons Learned When Evaluating the Feasibility of Emerging Green Technologies** (FrC4a)
Sean J. Dee, Russell A. Ogle (Exponent)
Many companies are looking for opportunities to utilize green technologies such as bioenergy or bio-based chemical production. There are many exciting developments in these fields, but the one key question is, ‘Is this technology feasible technically and economically?’ Successful commercialization depends on many disparate factors such as fundamental technology performance, availability of lab studies and pilot studies, environmental permitting issues, feedstock logistics, regulatory compliance, and economic analysis. The combination of all these factors will ultimately contribute to the final decision to invest time, resources, or personnel on continual development of the technology.
Exponent has been involved in assisting clients evaluate and understand these potential opportunities. During our experience, we have identified several key questions that help guide the analysis and assist our clients with the determination of project feasibility. This presentation will highlight the structured approach that is undertaken during the evaluation, and the role that engineers play when considering the technology, available data, economics, and logistics in order to determine the overall viability of a proposed project.

4:20 PM **Thermal Energy Storage Device for Space Cooling Applications** (FrC4b)
Siddique Khateeb, Mukund Bhaskar, Said Al-Hallaj (AllCell Tehcnologies)

HVAC (Heating, Ventilation and Cooling) accounts for approximately 15-30% of a commercial building's electricity cost and about 20-40% of electricity consumption. Electricity costs charged by the utilities companies for commercial building customers includes consumption charges ($/kWh) and demand charges ($/kW) depending on the time of use (TOU) charges. Thus, there is great interest to reduce the electricity consumption charges and demand charges by using new energy efficient technologies and products. One such product is a thermal energy storage (TES) system using a phase change material (PCM) to offset the cooling costs associated with air-conditioning systems by reducing the electricity consumption during peak time periods. Ice TES system have certain drawbacks such as low charge and discharge capability to transfer the cold energy, high operation costs. In order to overcome these drawbacks, a patented phase change composite (PCC) TES material is developed that has very high thermal conductivity and adjustable phase change temperature to increase the rate capability to transfer cold energy, lower system costs and reduce operational costs because of higher operating temperature than ice. Proof of concept demonstration and working prototype results of a PCC TES system have been successfully completed and the results show that a high rate capability PCC TES system can be designed for a commercial building with high efficiency at low and high discharge rates. Techno-economic analysis for peak shaving or peak load shifting of a commercial air-conditioning system was studied to compare Ice and PCC TES system. Results showed that a PCC TES system can be designed and manufactured to compete with Ice TES system with favorable ROI (return on investment).

4:40 PM **Developing and Analyzing Chemical Process Data for Life Cycle Inventories and Sustainability Evaluation** (FrC4c)
Gerado J. Ruiz-Mercado, Raymond L. Smith, Michael A. Gonzalez (US EPA)

Chemical industries have transformed the quality of human life rapidly by performing chemical and physical transformations of ecological goods and services to value products; most often without considering if those transformation routes, methods, or processes were sustainable or unsustainable.

The absence of sustainable practices has led to negative impacts to the environment and society. In addition, unsustainable practices have led to the fabrication of products without adequate or responsible end-of-use and/or disposal that would make them feasible for their recovery, recycling, or biodegradability.

Fortunately, this is being changed since society, government, and industry realized that sustainable practices have the potential for obtaining economic benefits without damaging the environment. There are many private and public initiatives regarding the implementation in practice of sustainable development. However, it is often unclear what the effects of these new practices are in the environment. In order to offer a more comprehensive description of environmental, social, and economic effects, the U.S. Environmental Protection Agency has proposed a web-based tool called GREENSCOPE (Gauging Reaction Effectiveness for the Environmental Sustainability of Chemistries with a multi-Objective Process Evaluator) to support decision makers when developing, designing, and evaluating sustainable processes and products. One of the main outcomes of GREENSCOPE is a life cycle inventory for synthesis routes and processes. The life cycle inventory is an important step in the development of life cycle assessments, which determine environmental effects throughout a product's life cycle stages, starting from resource extraction, through product manufacturing, distribution and use, and recycling or disposal.

GREENSCOPE evaluates sustainability of existing and new technologies by employing performance indicators for objectives in four main areas: environment, economics, energy, and efficiency. A case study demonstration using GREENSCOPE will be performed to provide decision makers guidance on using this assessment and design tool, from data entries to sustainability evaluation outcomes and the related life cycle inventory generation. The tool can then show which indicators have improved and where additional opportunities for improvement exist. The indicator scores describe product and process performance on a sustainability measurement scale, determining whether chemical products and processes are more or less sustainable. This contribution will present the GREENSCOPE tool as an approach to achieving life cycle assessments of chemical products during their manufacturing stages.

5:00 PM **Valuing Water in Rankine Cycle Power Generation** (FrC4d)
Suresh Jambunathan (Veolia)

The steam Rankine cycle is a proven method to generate power. The condenser sub-system is integral to power generation. However, executive attention is often directed towards the "exciting" components of the cycle – boiler, steam turbine etc… and the choice of condensing cycle is usually the last agenda item during the decision making process. Often, power companies may be leaving money on the table by sub-optimally choosing the condensing cycle.

A common economic and hence technical choice involves choosing between a Water Cooled Condensing (WCC) cycle versus an Air Cooled Condensing (ACC) cycle. Amongst the dozens of variables that impact the technical & economic choice, which variables are significant?

This presentation starts by overviewing macroeconomic trends – hotter & dryer weather conditions in specific geographies and

the looming impact of clean power policies impacting power generation.
It then discusses the effect of thermodynamic factors – throttle steam conditions, turbine efficiency, ambient wet & dry bulb temperatures on rankine cycle efficiency.
Finally it looks at the process via an economic prism - the incremental value of power versus the cost of water saved to help a power plant executive understand technical & economic trade-offs when contemplating power generation in a WCC or ACC mode.

5:20 PM **Prospective Life-cycle Technology Assessment Modeling Framework for Sustainable Chemical Production** (FrC4e)
Yuan Yao, Eric Masanet (Northwestern University), *Diane Graziano, Matthe Riddle* (Argonne National Laboratory), *Joe Cresko* (US DOE)

Assessing the energy, environmental, and economic impacts of emerging technologies for more sustainable chemical processes is critical because it provides policy makers with good references on future investment and technology promotion; it also provides manufacturers and researchers with a better understanding of technology potential, possible bottlenecks and future R&D directions. However, the assessment of new technologies is challenging for the lack of process data, general evaluation approaches across different products, and robust methodologies over the large temporal and spatial scales.
In this work, a multi-scale assessment modeling framework integrating chemical process design and modeling, life cycle assessment, and techno-economic analysis is presented. This model is able to generate missing process data for novel technologies by chemical process design and modeling, quantify the net impacts of emerging technologies on energy and emissions through life cycle assessment, make reasonable projections over temporal and spatial scales, and conduct scenario analysis to make robust conclusions.
A case study of cradle-to-gate ethylene production system is shown for demonstration. Ethylene is one of the largest energy consumer and greenhouse gas (GHG) emissions resources in the chemical industry [1, 2]. The rapid growth of ethylene production contributed by shale gas boom adds significant amount of energy consumption and GHG emissions to the chemical industry [3]. Intensive R&D efforts have been made to develop innovative technologies for improving energy efficiency or mitigating GHG emissions of the ethylene industry. The modeling framework was applied to the ethylene case study for assessing the impacts of new technologies and feedstock shifts on industrial energy consumption and GHG emissions of the ethylene production in future decades. The results indicate that energy consumption and GHG emissions of ethylene life cycle are highly driven by fugitive emissions coming from the upstream and thermal efficiency of several key unit operations such as furnace and separators [4]. New technologies working on improving these parameters have high chance to get promising potentials of energy and emissions reduction. For example, by 2040, a hybrid distillation technology can reduce 60 million GJ of life-cycle energy consumption of the U.S. ethylene industry and avoid 4 million tons of CO_2-equiv GHG emissions.
The results highlight the critical factors driving the energy consumption, GHG emissions and resource utilization of chemical production; they also shed light on opportunities for reducing energy and GHG emissions. The modeling framework provides a reliable methodology to overcome knowledge barriers and deliver robust insights of potential influences that emerging technologies can have at a very large scale. The model can be further coupled with assessment models for other environmental indexes to support decision making and to enhance strategic planning for meeting short-term and long-term sustainability goals at both the plant and industrial scales.

[1]. Y. Yao, D. Graziano, M. Riddle, J. Cresko, and E. Masanet, "Greener pathways for energy-intensive commodity chemicals: opportunities and challenges," Current Opinion in Chemical Engineering, vol. 6, pp. 90-98, 11// 2014.
[2]. IEA, ICCA, and DECHEMA, "Technology Roadmap, Energy and GHG Reductions in the Chemical Industry via Catalytic Process," IEA, ICCA, DECHEMA, France2013.
[3]. American Chemistry Council (ACC), "Year-end 2013 chemical industry situation and outlook," Washington, DC, USA2013.
[4]. Y. Yao, D. J. Graziano, M. Riddle, J. Cresko, and E. Masanet, "Understanding variability to reduce the energy and GHG footprints of U.S. ethylene production," Environmental Science & Technology, 2015/11/02 2015.

(Canceled) **Process Safety Workshop II**
~~Friday, March 4, 2016 (Crown Room, **FrC5**)~~
Chair: *Peter Hereña* (Baker Engineering and Risk Consultants, Inc.)
Co-Chair: *Brenton L. Cox* (Exponent Inc.)

(Canceled) 4:00 PM **Quantitative Risk Analysis** (FrC5a)
Jesse Calderon, Mike Toraason (Baker Engineering and Risk Consultants, Inc.)

Operating companies use consequence modeling to understand the onsite and offsite risk associated with release of flammable and toxic materials from chemical processes. Doing so helps a company provide countermeasures and controls that impacts to personnel.
The Quantitative Risk Analysis (QRA) method attempts to answer the following questions with respect to onsite and offsite releases: What can go wrong? How likely is it? What are the impacts? So what should I do? The approach utilizes a simple framework to quantify the impact of flammable and toxic releases. This quantification requires the assimilation of process information, site-specific data, offsite population densities, weather data, failure analysis and consequence modeling. The workshop will review basic terminology and describe how consequence modeling can be supplemented

with a QRA to understand the likelihood of consequences and the total risk posed by the facility operation. The workshop will also describe the information that is typically needed to perform such a study, and what process engineers and technicians must know to be able to understand QRA.

(Canceled) 4:55 PM **Standard Operating Procedures** (FrC5b)
Sunil Lakhiani, Sean Dee (Exponent Inc.)
Standard operating procedures (SOPs) are an integral part of process safety and a critical layer of defense in the process industry. SOPs provide detailed, step-by-step instructions to operators/employees to perform the job safely. Due to the importance of the role of SOPs in work situations, especially critical tasks, it is important to have procedures which are not just technically accurate, but are free of error traps that may increase the likelihood for human errors and can lead to undesirable outcomes. The purpose of this workshop is to identify various error inducing factors that need to be considered and resolved during the development and review of SOPs. In addition, the workshop will cover guidelines for developing procedures that enhance comprehension and reduce the potential for human errors.

AIChE Midwest Regional Conference

Conference Organizers

Conference Planning Chair

Pat Shannon (Middough)

AIChE National Liaison

Stephanie Orvoine-Couvrette (AIChE Headquarters)

General Arrangements Committee

- Finance Committee

Budget:	*Pat Shannon* (Middough)
Fundraising:	*Azita Ahmadzadeh* (UOP/Honeywell), *Janet Werner* (Middough)
Facilities:	*Ariana Mayorga* (EN Engineering)

- Advertising and Registration Committee

Online registration:	*Steve Wozniak* (Ambitech Engineering)
Onsite Registration:	*Jerry Wilks* (CITGO)
Website:	*Tom King* (UOP/Honeywell))

- HS Outreach Committee

HSO Committee Chair:	*Ellen Kloppenborg* (UOP/Honeywell)
HSO registration:	*Ellen Kloppenborg* (UOP/Honeywell)
HSO marketing:	*Tim Lipman* (Illinois Institute of Technology), *Jody Buck* (Illinois Institute of Technology),
HSO programming:	*Olha Zvarych* (Illinois Institute of Technology)
HSO volunteers:	*Badar Jarai* (Illinois Institute of Technology)

- Hospitality Committee

Hospitality Committee Chair:	*Roger Alexandre Ngosso*
YP social:	*Liam O'Rourke* (Fauske & Associates)
Lodging and travel:	*Roger Alexandre Ngosso*
Program book printing:	*Roger Alexandre Ngosso*
Student aid coordination:	*Badar Jarai* (Illinois Institute of Technology)

Programming Committee

Programming Chair:	*Donald Chmielewski* (Illinois Institute of Technology)
Programming Logistics:	*Liam O'Rourke* (Fauske & Associates), *Emily Kunkel* (Sargent & Lundy)
Poster Session:	*Satish Parulekar, Seok Hoon Hong* (Illinois Institute of Technology)

<u>Technical Programming Committees</u>

- Biomedical, Pharmaceutical and Nano-Engineering

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Salvador Garcia-Munoz	Eli Lilly
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- Process Safety and Occupational Health

Janet Grezlik (chair)	Process Safety and Reliability Group
Qingsheng (Sam) Wang	Oklahoma State University
Brenton Cox	Exponent
Peter Herena (past chair)	BakerRisk

- Refining and Petrochemical Processing

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Chenn Zhou	Purdue-Calumet
Jeffery Zalc	BP
Martin Gonzalez (past chair)	BP

AIChE Midwest Regional Conference

High School Outreach Program

8:30-9:15 **Engineering Expo** (Gallery Lounge)
- Meet with current engineering students and see some of their projects

9:15-10:45 Groups will split into two groups and rotate through the following 40 minute activities

Presentation on Engineering Careers (Auditorium)
- Learn about how engineers contribute to all aspects of society
  Presented by Bonnie Haferkamp (Illinois Institute of Technology)

Team Building Exercise (Expo Room)
- Work with other students to complete a hands-on engineering-related task

10:45-11:30 **Engineering Panel Session** (Auditorium)
- Learn about the day-to-day activities of practicing engineers and engineering students. Time to ask your most burning questions.

11:30-12:30 **Engineering Lunch** (Ballroom and Expo Room)
- Opportunity for one-on-one discussions with engineering professionals and students.

12:30-1:30 **Keynote Speaker** (Auditorium)
- Dr. Pete Ludovice – Comedian and Chemical Engineering Professor at Georgia Tech

1:30-2:30 **Tours of the Illinois Tech Campus** (Meet at Gallery Lounge)

This special high school program is being run in parallel with the American Institute of Chemical Engineers (AIChE) 8th Annual Midwest Regional Conference, the objective of which is to build technical relationships between industrial practitioners and governmental and academic researchers. AIChE and Illinois Tech would like to expose students to the profession of chemical engineering and engineering in general, and give them the opportunity to interact with professional engineers, engineering students, and faculty. We hope you come away from this program with some idea of what chemical engineers do, how they touch your life, and whether you would like to pursue an engineering career. We encourage you to stay engaged, ask questions, and have fun!

Dr. Pete Ludovice

The world's only touring comedian with a Ph.D. from M.I.T., Pete has performed internationally as a comedian for over a decade, and taught Georgia Tech Chemical Engineers for over two decades. His research activities include the computer modeling of synthetic and biological macromolecules, and the use of humor to improve technical innovation, communication, and education (ludovice.chbe.gatech.edu). One of his National Science Foundation projects examines the use of humor in engineering education. He co-directs the Humor Genome Project (humorgenome.org) and the Geekapalooza Comedy Tour (pwp.gatech.edu/geekapalooza) at Georgia Tech. Pete also hosts a weekly radio show on science and technology whose motto is "Science, only funnier" (WREK-Atlanta, 91.1FM, insidetheblackbox.org), and a podcast on the intersection of science and the humanities (www.peteandcharlie.libsyn.com/).

ACKNOWLEDGEMENTS

HS Outreach Organizing Committee

Chair: Ellen Kloppenborg (UOP)

Co-Chair Programming: Olha Zvarych (Illinois Institute of Technology)

Co-Chair Logistics: Bader Jarai (Illinois Institute of Technology)

HS Outreach Organizing Committee: Tim Lipman, Jody Buck, Don Chmielewski (Illinois Institute of Technology)

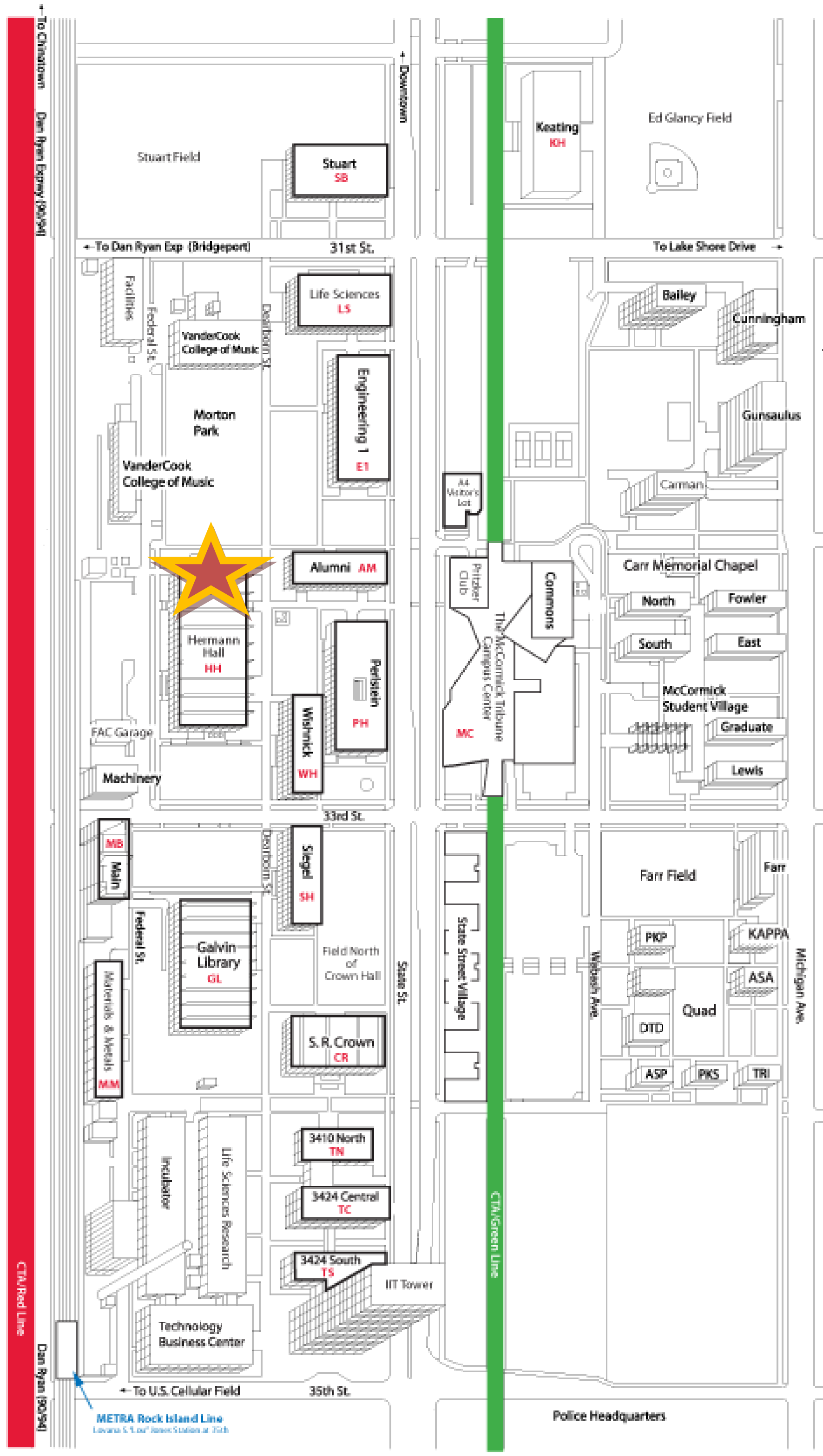
Program Emcee: Jaylen Taylor (Illinois Institute of Technology)

Conference Venue

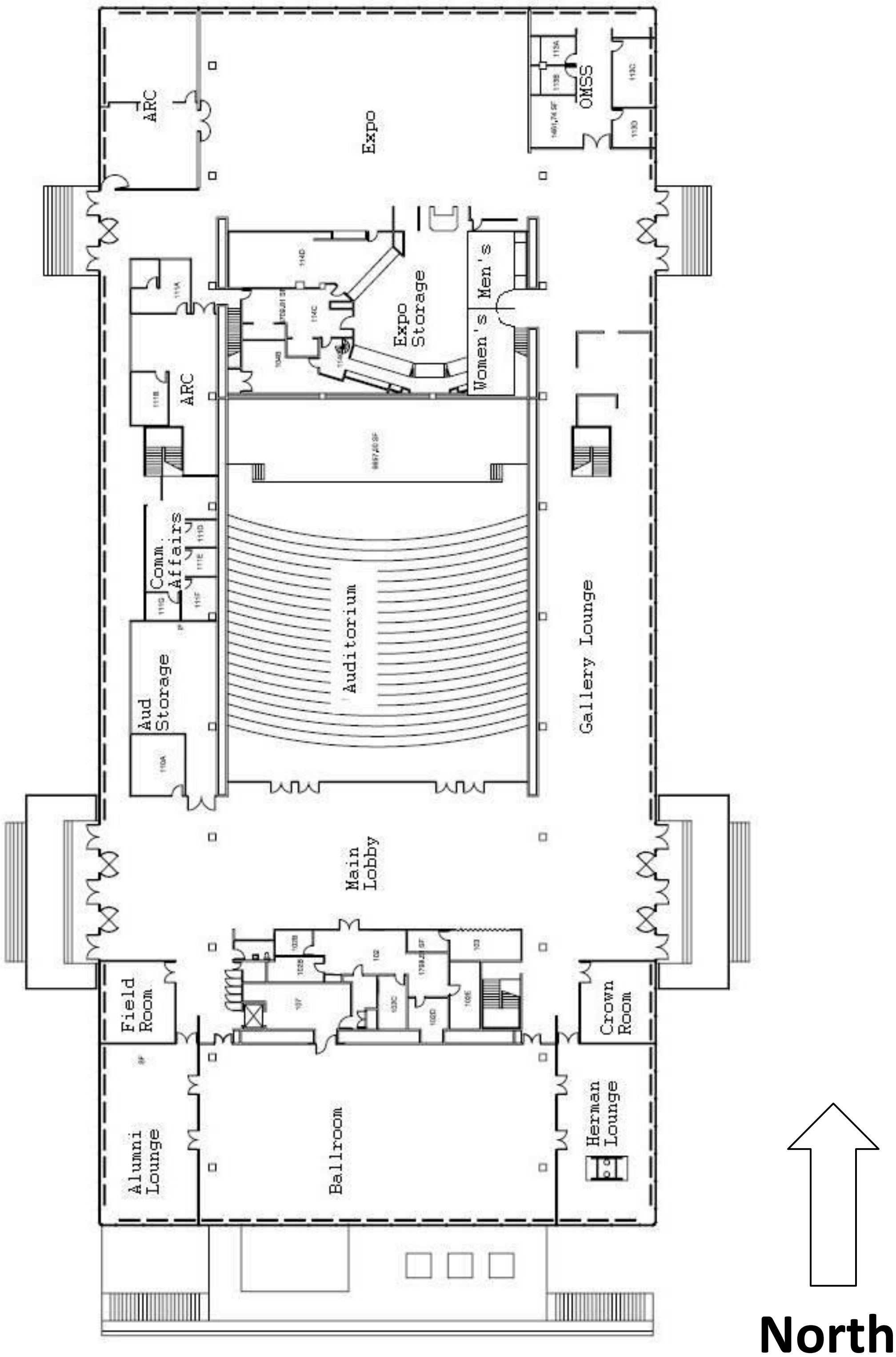
Hermann Hall

3241 S Federal St
Illinois Institute of Technology
Chicago, IL 60616

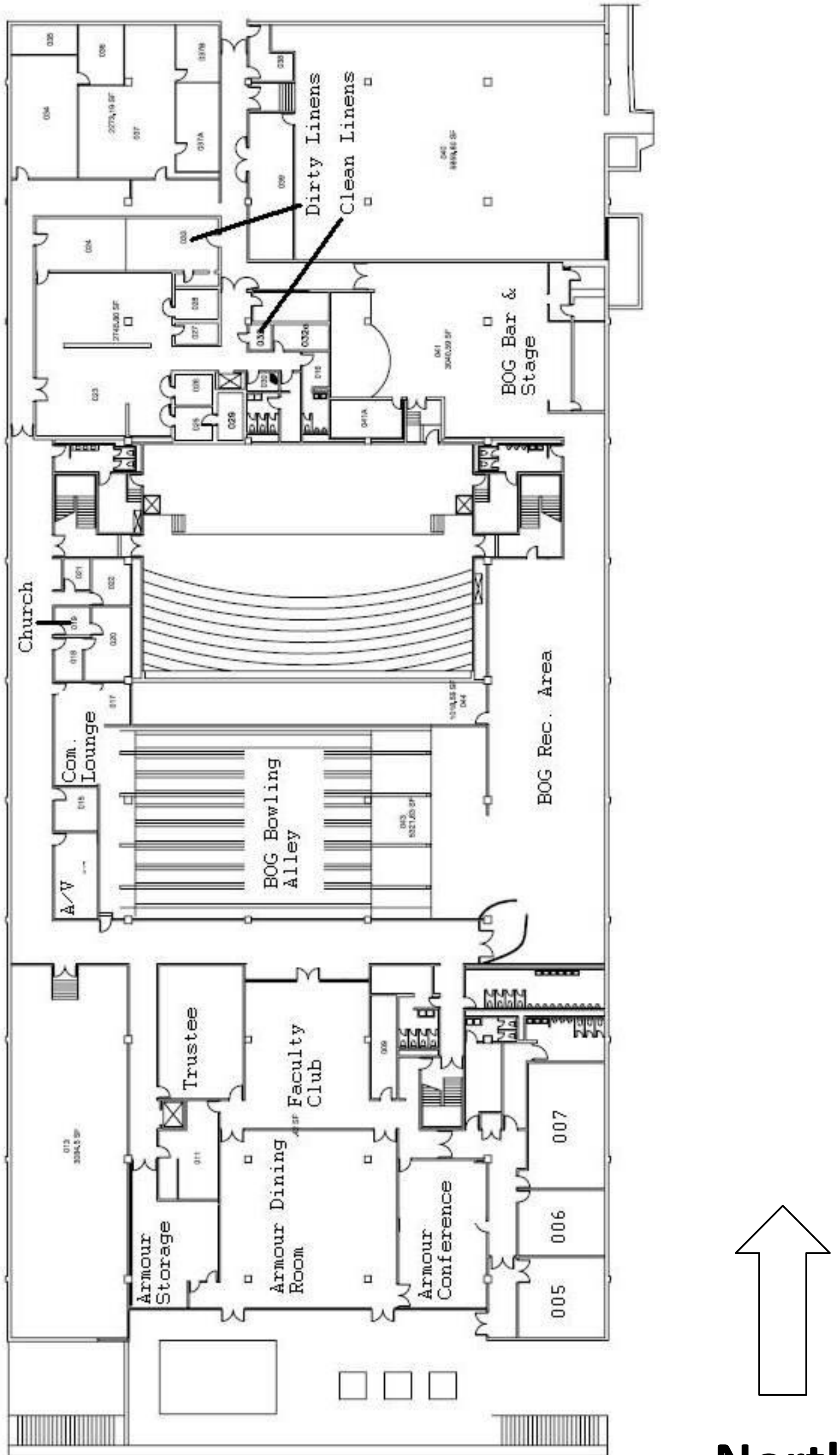
Useful Links:
Campus Map
Directions
Campus Parking
(MRC parking is available in lot B5, adjacent to HH)



Map of Herman Hall (first floor)



Map of Herman Hall (basement floor)



North

MRC 2017

9th Annual AIChE Midwest Regional Conference

Chicago - Spring 2017

For programming and volunteer opportunities please contact Professor Chmielewski at chmielewski@iit.edu

AIChE Midwest Regional Conference

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Please provide us your feedback about the 2016 MRC.

This 5-minute survey will help improve future conferences.

Use your Smartphone to scan this QR-code:

Or go to this website

http://tinyurl.com/MRC2016-feedback

AIChE Midwest Regional Conference

Young Professionals Networking Social

What: YP Social after the 8th Annual Midwest Regional Conference at IIT

When: Friday, March 4th 7:00 – 9:00 PM

Where: Rocky's Chicago

234 W 31st Street

Chicago, IL 60616

Soft drinks and appetizers provided courtesy of our YP Networking Event Sponsor, Reactor Resources

REACTOR RESOURCES

Hosted by AIChE Chicago Young Professionals Committee (YPC)