AIChE®
MIDWEST REGIONAL CONFERENCE

10th Annual
AIChE Midwest Regional Conference

March 13-14, 2018
Illinois Institute of Technology
(Hermann Hall)

Organized by the AIChE Chicago Local Section and hosted by the Illinois Institute of Technology

Armour College of Engineering
ILLINOIS INSTITUTE OF TECHNOLOGY

AIChE Chicago

AIChE Midwest Regional Conference

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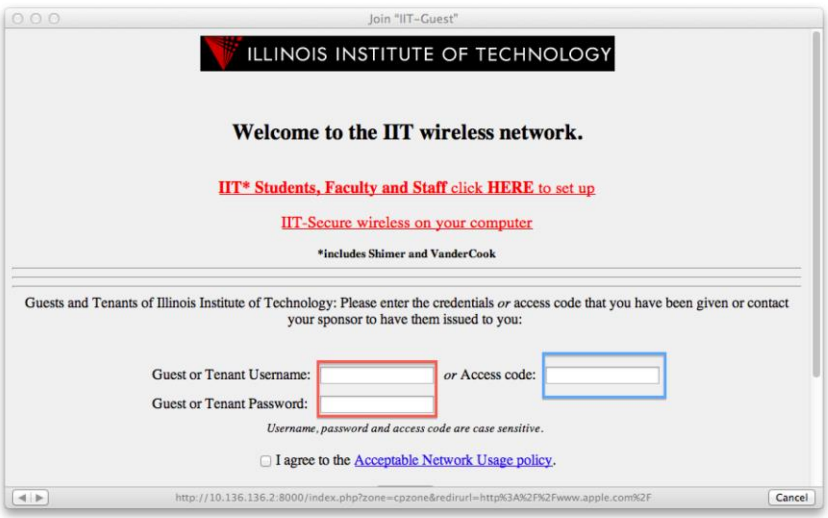

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AIChE Midwest Regional Conference

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AIChE Midwest Regional Conference

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 10th 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. The technical program includes:

<u>3 Keynote Lectures</u>:

- **Jim Rekoske**, Chief Technology Officer, UOP/Honeywell
- **John A. Rodgers**, Professor/Director, Center on Bio-Integrated Electronics, Northwestern University
- **Doraiswami Ramkrishna***, Distinguished Professor, Purdue University*

<u>4 Plenary Lectures</u>:

- **Russell A. Ogle**, *Principal Engineer, Exponent*
- **Christopher W. Jones,** Professor/Associate Vice President for Research, Georgia Tech
- **Thomas Foust,** Director, National Bioenergy Center, NREL
- **Kimberly Gray**, *Professor and Chair, Civil and Environmental Engineering, Northwestern University*

There are **18 technical sessions** featuring over **50 oral presentations** over the 2 days of the conference as well as **6 career development sessions**. The Wednesday evening program is combined with the ***AIChE Chicago Local Section Monthly Meeting***.

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 **Valarie King–Bailey** (CEO, OnShore Technology Group) as keynote speaker and includes a special luncheon where students can interact with practicing chemical engineers.

On behalf of the conference planning committee, we welcome you to the 10th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Reza Mostofi
Conference Chair
UOP/Honeywell

AIChE Midwest Regional Conference

Program at a Glance

Tuesday, March 13, 2018

7:30 AM - 10:30 AM	**Continental Breakfast** (Faculty Club)
8:45 AM – 10:00 AM	**Morning Keynote** (HH 002) *- Jim Rekoske, UOP/Honeywell*
10:00 AM – 10:15 AM	**Networking Break**
10:15 AM – 11:30 AM	**Technical Sessions** - *Process Safety I* (HH 002) - *Reaction Engineering* (HH 005) - *Tutorial Session: Particulate Processing* (HH 003) - *Panel Session: Work/Family Life Balance* (HH 010)
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** - *Russell A. Ogle, Exponent* (HH 002) - *Christopher W. Jones, Georgia Tech.* (HH 005)
1:45 PM – 2:00 PM	**Networking Break**
2:00 PM – 3:15 PM	**Technical Sessions** - *Process Safety II* (HH 002) - *Catalysis I* (HH 005) - *Modeling of Biological Processes* (HH 003) - *YP Workshop: Entry Level ChE Experiences* (HH 010)
3:15 PM – 3:30 PM	**Networking Break**
3:30 PM – 4:45 PM	**Technical Sessions** - *Refining & Petrochemical Processing* (HH 002) - *Catalysis II* (HH 005) - *Tissue Engineering* (HH 003) - *Panel Session: Dealing with Difficult Co-Workers* (HH 010)
4:45 PM – 5:00 PM	**Networking Break**
5:00 PM – 6:30 PM	**Poster Session** (Gallery Lounge) [**canceled**]
5:00 PM – 8:00 PM	**YP Social** (HH Bog)

AIChE Midwest Regional Conference
Program at a Glance

Wednesday, March 14, 2018

7:30 AM - 10:30 AM	**Continental Breakfast** (Faculty Club)
8:45 AM – 10:00 AM	**Morning Keynote** (HH 002) - *John A. Rodgers, Northwestern University*
10:00 AM – 10:15 AM	**Networking Break**
10:15 AM – 11:30 AM	**Technical Sessions** - *Process Engineering* (HH 002) - *Bio-Medical Engineering I* (HH 005) - *Bio-Interfaces* (HH 003) - *Panel Session: They Just Made Me Team Leader: Now What Do I Do?* (HH 010)
11:30 AM – 12:30 PM	**Lunch with High School Outreach Participants** (Illinois A and Illinois B)
12:45 PM – 1:45 PM	**Afternoon Plenary Sessions** - *Thomas Foust, National Bioenergy Center, NREL* (HH 002) - *Kimberly Gray, Northwestern University* (HH 005)
1:45 PM – 2:00 PM	**Networking Break**
2:00 PM – 3:15 PM	**Technical Sessions** - *Electro-chemical Engineering* (HH 002) - *Bio-Medical Engineering II* (HH 005) - *Transport Phenomena I* (HH 003) - *Tutorial Session: Basic Mixing and Baffling* (HH010) - *YP Workshop: Mock Interviews* (HH 007)
3:15 PM – 3:30 PM	**Networking Break**
3:30 PM – 4:45 PM	**Technical Sessions** - *Bio-Based Products and Fuels* (HH 002) - *Bio-Medical Engineering III* (HH 005) - *Transport Phenomena II* (HH 003) - *Workshop: Job Search Essentials* (HH 010)
4:45 PM – 5:00 PM	**Networking Break**
5:00 PM – 6:00 PM	**Local Section Dinner Reception** (Ballroom)
6:00 PM – 7:00 PM	**Local Section Dinner** (Ballroom)
7:00 PM – 8:00 PM	**Dinner Keynote** (Ballroom) - *Doraiswami Ramkrishna, Purdue University*

AIChE Midwest Regional Conference
Keynote and Plenary Speakers

Tuesday Morning Keynote: 8:15 AM March 13, 2018

Jim Rekoske*, Chief Technology Officer, UOP/Honeywell*

Presentation Title: **Light Hydrocarbon Conversion Chemistry Challenges in an Era of Abundant Supply of Raw Material**

Biographical Sketch: *Jim Rekoske is Vice President and Chief Technology Officer at UOP Honeywell. In this role, he is responsible for the entire technology organization, ranging from basic and applied research on new materials, catalysts, membranes and adsorbents through to process development, scale-up and commercialization. Previously, Jim served as Technical Director for Petrochemical Catalysts, Director of Technology for Universal Pharma Technologies and Vice President & General Manager of UOP's Renewable Energy & Chemicals business unit. Immediately prior, he was the Global Business Director for UOP's petrochemical business segment. Jim was awarded the 2010 Herman Pines Award from the Chicago Catalysis Club. He is a member of the advisory boards for the C3Bio Center of Excellence at Purdue University, the School of Chemical Engineering at Purdue University, and the College of Engineering at the University of Wisconsin-Madison. Jim earned his BS and MS degrees in chemical engineering at the University of Wisconsin and his PhD in chemical engineering from the University of Delaware. He also earned an MBA from the Booth School of Business at the University of Chicago.*

Tuesday Afternoon Plenary Session I: 12:45 PM March 13, 2018

Russell A. Ogle, *Principal Engineer, Exponent*

Presentation Title: **Dust Explosion Dynamics: Combustion Theory as a Bridge to Better Safety Management**

Biographical Sketch: *Dr. Russell Ogle is a Principal Engineer and the Practice Director for Thermal Sciences at Exponent. He specializes in the scientific investigation and prevention of complex industrial accidents and catastrophic fires and explosions. He received his B.S in Chemical Engineering from Purdue University and a Ph.D. in Chemical Engineering from the University of Iowa. He has 30 years of industrial experience working in fire, explosion, and chemical safety. Dr. Ogle is a licensed professional engineer, a certified safety professional, and a certified fire and explosion investigator. His new book, "Dust Explosion Dynamics," is an introduction to the combustion science of dust explosions and fires*

Tuesday Afternoon Plenary Session II: 12:45 PM March 13, 2018

Christopher W. Jones, *Professor and Associate Vice President for Research, Georgia Tech*

Presentation Title: **Amine-Modified Silicates as CO2 Sorbents and Catalysts**

Biographical Sketch *Professor Jones is the Love Family Professor of Chemical & Biomolecular Engineering and Associate Vice President for Research. Dr. Jones leads a research group that works in the broad areas of materials, catalysis and adsorption. Since joining Georgia Tech, he has been recognized with a number of awards for his research and teaching. The American Chemical Society recognized his catalysis research with the Ipatieff Prize in 2010, followed by the North American Catalysis Society with the Paul H. Emmett Award in Fundamental Catalysis in 2013. In 2016, he was recognized by the AIChE for his work in catalysis and CO2 capture with the Andreas Acrivos Award for Professional Progress. Dr. Jones is the founding Editor-in-Chief of the new journal, ACS Catalysis, which was recognized with the 2012 Prose Award as the Best New Journal in Science, Technology or Medicine, by the American Association of Publishers. As Associate Vice-President for Research, Jones is responsible for leading and managing interdisciplinary research activities across six colleges, the Georgia Tech Research Institute, and the Enterprise Innovation Institute.*

AIChE Midwest Regional Conference
Keynote and Plenary Speakers

Wednesday Morning Keynote: 8:15 AM March 14, 2018

John A. Rodgers*, Professor, Northwestern University*

Presentation Title: **Microfluidic Systems for the Skin**

Biographical Sketch: *Professor John A. Rogers obtained BA and BS degrees in chemistry and in physics from the University of Texas, Austin, in 1989. From MIT, he received SM degrees in physics and in chemistry in 1992 and the PhD degree in physical chemistry in 1995. From 1995 to 1997, Rogers was a Junior Fellow in the Harvard University Society of Fellows. He joined Bell Laboratories as a Member of Technical Staff in the Condensed Matter Physics Research Department in 1997, and served as Director of this department from the end of 2000 to 2002. He then spent thirteen years on the faculty at University of Illinois, most recently as the Swanlund Chair Professor and Director of the Seitz Materials Research Laboratory. In 2016, he joined Northwestern University as the Louis Simpson and Kimberly Querrey Professor of Materials Science and Engineering, Biomedical Engineering and Medicine, with affiliate appointments in Mechanical Engineering, Electrical and Computer Engineering and Chemistry. He serves as director of the newly endowed Center on Bio-Integrated Electronics.*

His research has been recognized by many awards including a MacArthur Fellowship (2009), the Lemelson-MIT Prize (2011) and the Smithsonian Award for American Ingenuity in the Physical Sciences (2013). He is a member of the National Academy of Engineering, the National Academy of Sciences, the National Academy of Inventors and the American Academy of Arts and Sciences.

Wednesday Afternoon Plenary Session I: 12:45 PM March 14, 2018

Thomas Foust, *Director, National Bioenergy Center, NREL*

Presentation Title: **Future Scenarios for Renewable Transportation Fuels in a Rapidly Changing Transportation Industry**

Biographical Sketch: *Dr. Thomas Foust is the Director of the National Renewable Energy Laboratory's National Bioenergy Center (NBC), a world leading organization of approximately 200 engineering and scientific staff performing cutting edge work to develop cost effective, environmentally sustainable technology for producing transportation fuels and products from biomass by delivering innovative, cost-effective biofuels and bio-products solutions. Dr. Foust is a comprehensive expert in the clean energy area with a specialty in bioenergy with over 25 years of R&D and R&D management experience. His areas of expertise in bioenergy include feedstock production, biomass conversion technologies to fuels and products and advantaged uses of biofuels and bio-products. Additionally, he has worked extensively in environmental and societal sustainability issues associated with clean energy. He has over 100 publications in the clean energy field covering numerous aspects of R&D, techno-economic analysis and environmental sustainability. Dr. Foust has a Ph.D. in Mechanical Engineering from the University of Idaho, a M.S. in Mechanical Engineering from the Johns Hopkins University, and a B.S. in Mechanical Engineering from the Pennsylvania State University. He is a licensed Professional Engineer.*

Wednesday Afternoon Plenary Session II: 12:45 PM March 14, 2018

Kimberly Gray, *Professor and Chair, Civil and Environmental Engineering, Northwestern University*

Presentation Title: ***Unexpected Behavior of Photoactive Nanocomposites in Energy & Environmental Applications***

Biographical Sketch: *Gray's areas of expertise are environmental catalysis and physicochemical processes in natural and engineered environmental systems with particular focus on energy and urban sustainability applications. She studies the synthesis, characterization and performance of photo-active materials, principally TiO2-based nanocomposites for solar fuel production and water/air treatment. Work in her group also involves the investigation of chemical fate in natural systems. She probes the role of periphyton (algal biofilms) in contaminant accumulation in stream sediments and in denitrification in wetlands. She studies the ways in which detailed understanding of ecological relationships (periphyton structure, dynamic food web descriptions) improves our ability to predict chemical transfer (bioaccumulation) in aquatic systems and ultimately human health risks. Application of this research is important in efforts to restore critical ecosystems (Great Lakes), to make ecological forecasts in the face of climate change and to employ ecosystem function for environmental protection (treatment wetlands). She is also studying the unintended ecotoxicological impacts of nanomaterials in aquatic systems. Recent work entails the adaptive design of urban systems to incorporate coupled ecological processes in response to climate change and demographic shifts. She works closely with the Chicago Legal Clinic to provide technical expertise to solve environmental problems for low-income urban communities and with other NGO in the Chicago region to develop creative solutions for resource recovery and economic recovery. She was a Senior Science Fellow at the Environmental Law and Policy Center. She is the author of over 100 scientific papers and lectures widely on energy, climate and environmental issues.*

Wednesday Dinner Keynote: 6:30 PM March 14, 2018

Doraiswami Ramkrishna*, Distinguished Professor, Purdue University*

Presentation Title: **Metabolic Complexity. Is there Music Behind it?**

Biographical Sketch: *Doraiswami Ramkrishna, popularly known as Ramki, obtained his Bachelor's degree in Chemical Engineering in 1960 from the Bombay University Department of Chemical Technology, now known as ICT. He received his PhD in 1965 from the University of Minnesota, and after serving for two years on the faculty at Minnesota, returned to India to join the IIT Kanpur as an Assistant Professor. In 1974, he went back to the United States as a Visiting Associate Professor at the University of Wisconsin and as a Visiting Professor the following year at the University of Minnesota before joining the Purdue University faculty in 1976 as a full Professor. In 1994, he was appointed H.C. Peffer Distinguished Professor. Professor Ramkrishna is noted for his research on the application of mathematics to chemical and biochemical reaction engineering, biotechnology, particulate systems, and more recently personalized medicine. He is well known for the book Linear Operator Methods in Chemical Engineering (Prentice-Hall, 1985) coauthored with Neal Amundson, and his book Population Balances. Theory and Application to Particulate Systems in Engineering (Academic Press, 2000).*

He is a recipient of several AIChE Awards, the Alpha Chi Sigma (1987), the Richard Wilhelm Award (1998), the Thomas Baron Award (2004). He is a Fellow of professional societies, American Institute of Medical and Biological Engineering (1996), and of the American Institute of Chemical Engineers (2008). From Germany, he won the Senior Humboldt Award (2001) to visit the Max Planck Institute in Magdeburg. Bombay University honored him with the UDCT Diamond Award (1994), the Platinum Award (2009) and Ruia College with the Jewel of Ruia Award. Professor Ramkrishna has held several Distinguished Professorships and delivered numerous Distinguished Lectures. In (2009) he was elected to the US National Academy of Engineering, and as a foreign member to the Indian National Academy of Engineering in 2011.

AIChE Midwest Regional Conference
Session Presentations
Tuesday, March 13, 2018

Tuesday Morning Keynote Session
Tuesday, March 13, 2018 (HH 002)
8:45 AM **LS Chair's Welcome**
Janet Werner (Middough)
8:55 AM **Keynote Introduction**
Adam Kanyuh (UOP / Honeywell)
9:00 AM **Light Hydrocarbon Conversion Chemistry Challenges in an Era of Abundant Supply of Raw Material**
Jim Rekoske (UOP / Honeywell)

Process Safety I
Tuesday, March 13, 2018 (HH 002, **TueA1**)
Chair: *Robert Weber* (PSRG)
10:15 AM **The Sweet Smell of Ammonia Hazards** (TueA1a)
Nicholas Train, Sean Dee, Brenton L. Cox (Exponent)
10:40 AM **Mitigation of Flammable and Toxic Hazards through Facility Design: Beyond Code Minimums** (TueA1b)
Craig Vesely, Bryan Haddon, Matt Austin (Affiliated Engineers, Inc.)
11:05 AM **PHA facilitation and how it dovetails with negotiation techniques** (TueA1c)
Herena, Peter (Baker Risk)

Reaction Engineering
Tuesday, March 13, 2018 (HH 005, **TueA2**)
Chair: *Mohammad Asadi* (Illinois Tech)
10:15 AM **Effect of Phosphate Salts and Solution pH in the Aqueous-phase Homo and Co-polymerization of NVP** (TueA2a)
Fernando Borges, Fouad Teymour (Illinois Tech)
10:40 AM **Imidazolinium Based Porous Hypercrosslinked Ionic Polymers for Efficient CO2 Capture and Fixation with Epoxides** (TueA2b)
Jing Li, Jiahua Zhu (University of Akron), *Jun Wang, Yu Zhou* (Nanjing Tech University)
11:05 AM **Design of the Next Generation Polymerization Reactor using CFD** (TueA2c)
Dimitri Gidaspow (Illinois Tech)

Tutorial Session: Particulate Processing
Tuesday, March 13, 2018 (HH 003, **TueA3**)
Chair: *Reza Mostofi* (UOP / Honeywell)
Co-Chair: *Donald Chmielewski* (Illinois Tech)
10:15 AM **What's a Particle?** (TueA3a)
Ben Freireich (Particulate Solid Research, Inc.)

Panel Session: Work/Life Balance
Tuesday, March 13, 2018 (HH 010, **TueA4**)
Chair: *Jaylen Taylor* (City of Chicago Dept of Water Management)
10:15 AM **Two Parents, Two Careers – Where Do They Find the Time** (TueA4a)
Jim Rekoske (UOP/Honeywell), *Linda Broadbelt* (Northwestern University), *Hakim Iddir* (Argonne National Laboratory), *Hadjira Iddir* (UOP/Honeywell)

Tuesday Plenary Session I
Tuesday, March 13, 2018 (HH 002)
12:45 PM **Plenary Introduction**
Brenton L. Cox (Exponent)
12:55 PM **Dust Explosion Dynamics: Combustion Theory as a Bridge to Better Safety Management**
Russell A. Ogle (Exponent)

Tuesday Plenary Session II
Tuesday, March 13, 2018 (HH 005)
12:45 PM **Plenary Introduction**
Fouad Teymour (Illinois Tech)
12:55 PM **Amine-Modified Silicates as CO2 Sorbents and Catalysts**
Christopher W. Jones (Georgia Tech)

Process Safety II
Tuesday, March 13, 2018 (HH 002, **TueB1**)
Chair: *Brenton L. Cox* (Exponent)
2:00 PM **O2 No! - Safety Considerations for Oxidation Reactions** (TueB1a)
Miguel E. Garcia, Brenton L. Cox, Sean Dee (Exponent)
2:25 PM **Process Safety – Leading key performance indicators** (TueB1b)
Scott M Wozniak (UOP/Honeywell) [**canceled**]
2:50 PM **Defining "Adequate" in Adequate Ventilation** (TueB1c)
Matthew S. Walters, Sean Dee, Brenton L. Cox (Exponent)

Catalysis I
Tuesday, March 13, 2018 (HH 005, **TueB2**)
Chair: *Masoudeh Ahmadi* (University of Louisville)
2:00 PM **Effect of Pt, Mo, Fe, Mg and Ni Promoters on Al2O3-CeO2 Catalyst for Oxidative Dehydrogenation of methane with Carbon Oxide** (TueB2a)

Abbas Jawad, Fateme Rezaei, Ali A. Rownaghi (Missouri University of Science and Technology) [**canceled**]

2:25 PM **Enhancing Energy Efficiency in Saccharide-HMF Conversion with Core/shell Structured Microwave Responsive Catalysts** (TueB2b)
Tuo Ji, Jiahua Zhu (University of Akron)

2:50 PM **Electrochemistry and Structure of Doped Li2FeSiO4/C Material as a Cathode for Li-ion Batteries** (TueB2c)
Kamil Kucuk, Carlo U. Segre, Elena V. Timofeeva (Illinois Tech)

Modeling of Bio and Pharmaceutical Processes

Tuesday, March 13, 2018 (HH 003, **TueB3**)
Chair: *Fatemeh Ostadhossein* (University of Illinois at Urbana-Champaign)

2:00 PM **Agent-Based Modeling of Mammalian Cell Culture** (TueB3a)
Robert Jackson, Ali Cinar (Illinois Tech)

2:25 PM **A Spatiotemporal Model Reveals Self-Limiting Receptor Crosslinking by Multivalent Antigens** (TueB3b)
Dipak Barua, Md Shahinuzzaman (Missouri University of Science and Technology)

2:50 PM **A Study of Residence Time Distribution and Continuous Crystallization in a Dynamic Baffle Mixed-Suspension-Mixed-Product-Removal Crystallizer** (TueB3c)
Claire Y. Liu (Purdue University), Alastair Barton, Paul Firth (AWL), *Jonathon Speed* (Keit Spectrometers) [**canceled**]

YP Workshop: Entry Level ChE Experiences

Tuesday, March 13, 2018 (HH 010, **TueB4**)
Chair: *Larry Avtzis* (CB&I)
Co-Chair: *Kimberly Douglas* (Abbott)

2:00 PM **Reading and Cross-Referencing a P&ID** (TueB4a)
Larry Avtzis (CB&I)

2:25 PM **Tales of a Quality Tech with an Engineering Degree** (TueB4a)
Kimberly Douglas (Abbott)

Refining and Petrochemical Engineering

Tuesday, March 13, 2018 (HH 002, **TueC1**)
Chair: *Jeffrey Zalc* (BP)
Co-Chair: *Hadjira Iddir* (UOP/Honeywell)

3:30 PM **Failures of Tubes in a Refinery Coker Furnace Due to Carburization** (TueC1a)
Gerald W. Wilks (CITGO Petroleum Inc.) [**canceled**]

3:55 PM **Fluidized Bed Stripper Hydrodynamics for Grating and Disk and Donut Trays** (TueC1b)
Allan S. Issangya, S.B. Reddy Karri, T. Knowlton, R. A. Cocco, B. Freireich (Particulate Solid Research, Inc.)

4:20 PM **Simplifying Hydrogen Production** (TueC1c)
Alec Rockwell (Johnson Matthey)

Catalysis II

Tuesday, March 13, 2018 (HH 005, **TueC2**)
Chair: *Fernando Borges* (Illinois Tech)

3:30 PM **Fabrication of Single Phased Iron Carbide Nanoparticles and Derived Heterostructures as Catalysts for Fischer-Tropsch Synthesis (FTS)** (TueC2a)
Ce Yang (Argonne National Laboratory)

3:55 PM **Structural Studies of Capacity Activation and Reduced Voltage Fading in Li-Rich, Mn-Ni-Fe Composite Oxide Cathode** (TueC2b)
Shankar Aryal, Carlo U. Segre, Elena V. Timofeeva (Illinois Tech)

4:20 PM **Production of Functionalized Carbon from Lignocellulosic Biomass** (TueC2c)
Masoudeh Ahmadi (University of Louisville)

Tissue Engineering

Tuesday, March 13, 2018 (HH 003, **TueC3**)
Chair: *Robert Jackson* (Illinois Tech)

3:30 PM **Cell Growth on Microparticles for Skin Tissue Engineering** (TueC3a)
Sutapa Barua (Missouri University of Science and Technology)

3:55 PM **3D Simulation of Bone Regeneration using Repast HPC: Optimal Scaffold Design for Bone Tissue engineering applications** (TueC3b)
Chenlin Lu, Mustafa C. Ozturk, Sami Somo, Eric M.Brey, Ali Cinar (Illinois Tech), *Banu Akar* (Northwestern University)

4:20 PM **Personalized Absorbable Gastrointestinal Stents for Intestinal Fistulae and Perforations** (TueC3c)
Parinaz Fathi, Fatemeh Ostadhossein, Indu Tripathi, Santosh K. Misra, Dipanjan Pan (University of Illinois at Urbana-Champaign), *Blair Rowitz* (Carle Foundation Hospital)

Panel Session: Interpersonal Skills

Tuesday, March 13, 2018 (HH 010, **TueC4**)
Chair: *Ignasi Palou-Rivera* (AIChE RAPID Manufacturing Institute)

3:30 PM **Dealing with Difficult Co-Workers** (TueA4a)
Derek Griffin (LanzaTech), *Barbara Padlo* (BP)

Poster Session

Tuesday, March 13, 2018 (Gallary Lounge)
5:00 – 6:30 PM **Poster Session**
[**canceled**]

AIChE Midwest Regional Conference

Session Presentations

Wednesday, March 14, 2018

<u>Wednesday Morning Keynote Session</u>
Wednesday, March 14, 2018 (HH 002)
8:45 AM **Recognition for Volunteers**
Reza Mostofi (UOP/Honeywell)
8:55 AM **Keynote Introduction**
Ali Cinar (Illinois Tech)
9:00 AM **Microfluidic Systems for the Skin**
John A. Rodgers (Northwestern University)

<u>Process Engineering</u>
Wednesday, March 14, 2018 (HH 002, **<u>WedA1</u>**)
Chair: *Juan Garcia* (Argonne National Laboratory)
10:15 AM **Introduction to the RAPID Manufacturing Institute, Program Roadmapping and First Projects** (WedA1a)
Ignasi Palou-Rivera (AIChE RAPID Manufacturing Institute)
10:40 AM **Bring it All Back to Nature: A New Paradigm in Environment-Energy-Nutrient Nexus** (WedA1b)
Meltem Urgun-Demirtas (Argonne National Laboratory)
11:05 AM **Design of Smart Grid Responsive Energy Storage Systems** (WedA1c)
Oluwasanmi Adeodu, Donald Chmielewski (Illinois Tech)

<u>Bio-Medical Engineering I</u>
Wednesday, March 14, 2018 (HH 005, **<u>WedA2</u>**)
Chair: *Dipak Barua* (Missouri University of Science and Technology)
10:15 AM **Nanosalina: A Tale of Saline-Loving Algae from the Lake's Agony to Cancer Therapy** (WedA2a)
Fatemeh Ostadhossein, Dipanjan Pan, Santosh Misra (University of Illinois Urbana Champaign)
10:40 AM **Cancer Cells as Signaling Factories** (WedA2b)
Mi Zhang, Harihara Baskaran, Roshini Balan, Reed Momjian (Case Western Reserve University)
11:05 AM **Colicin Production using Cell-free Protein Synthesis to Control Persister Cell Formation** (WedA2c)
Xing Jin, Seok Hoon Hong (Illinois Tech)

<u>Bio-Interfaces</u>
Wednesday, March 14, 2018 (HH 003, **<u>WedA3</u>**)
Chair: *Yongbeom Seo* (University of Illinois at Urbana-Champaign)
10:15 AM **Probiotic Escherichia Coli Outcompetes Pathogens during Biofilm Formation** (WedA3a)
Kuili Fang, Seok Hoon Hong (Illinois Tech), *Shweta Shree* (Birla Institute of Technology)
10:40 AM **Photopolymerization Techniques to Design Biomimetic, Micro-structured Interfaces** (WedA3b)
Caroline Szczepanski (Northwestern University)
11:05 AM **Temperature-dependent Synthesis of Multicolored Carbon Dots with Inherent Surface-Abundant Functionalities** (WedA3c)
Parinaz Fathi, Indrajit Srivastava, Santosh K. Misra, Dipanjan Pan (University of Illinois at Urbana-Champaign)

<u>Panel Session: Leadership Skills</u>
Wednesday, March 14, 2018 (HH 010, **<u>WedA4</u>**)
Chair: *Jeffrey Zalc* (BP)
10:15 AM **They Just Made Me Team Leader: Now What Do I Do?** (WedA4a)
Saadet Achigoz (UOP-Honeywell), *Kyle Kostroski* (BP), *Mike Schultz* (PTI Global Solutions), *Earl Washington* (South Chicago Packing)

<u>Wednesday Plenary Session I</u>
Wednesday, March 14, 2018 (HH 002)
12:45 PM **Plenary Introduction**
Mike Schultz (PTI Global Solutions)
12:55 PM **Future Scenarios for Renewable Transportation Fuels in a Rapidly Changing Transportation Industry**
Thomas Foust (National Bioenergy Center, NREL)

<u>Wednesday Plenary Session II</u>
Wednesday, March 14, 2018 (HH 005)
12:45 PM **Plenary Introduction**
Amid Khodadoust (University of Illinois at Chicago)
12:55 PM **Unexpected Behavior of Photoactive Nanocomposites in Energy & Environmental Applications**
Kimberly Gray (Northwestern University)

<u>Electro-chemical Engineering</u>
Wednesday, March 14, 2018 (HH 002, **<u>WedB1</u>**)
Chair: *Hakim Iddir* (Argonne National Laboratory)
2:00 PM **Lattice Templating and Galvanic Coupling Effects on the Electrochemical Performance of Core/shell Battery Materials** (WedB1a)
Elahe Moazzen, Elena Timofeeva, Carlo Segre (Illinois Tech)
2:25 PM **Transition Metal Segregation and Phase Transformations on the Surfaces of Layered Li(Ni1-x-yMnxCoy)O2 (NMC) Cathode Materials for Li-ion Batteries** (WedB1b)

Juan Garcia, Javier Bareno, Jason Croy, Hakim Iddir (Argonne National Laboratory), *Guoying Chen* (Lawrence Berkeley National Laboratory)

2:50 PM **In Situ EXAFS-derived Reversible Capacity Mechanisms in Sn-based Graphite Composite Anodes** (WedB1c)
Yujia Ding, Elena V. Timofeeva, Carlo U. Segre (Illinois Tech)

Bio-Medical Engineering II
Wednesday, March 14, 2018 (HH 005, **WedB2**)
Chair: *Sutapa Barua* (Missouri University of Science and Technology)

2:00 PM **Engineering Bioactive Hydrogels for Cardiac Repair** (WedB2a)
Arghya Paul (University of Kansas)

2:25 PM **Agent-Based Modeling of the interactions between lymphocytes and Beta cells in Type 1 Diabetes** (WedB2b)
Qian Xu, Mustafa Cagdas Ozturk, Ali Cinar (Illinois Tech)

2:50 PM **Active Antioxidizing Polymeric Particles for On-demand Pressure-driven Molecular Release** (WedB2c)
Yongbeom Seo, Hyunjoon Kong (University of Illinois at Urbana-Champaign)

Transport Phenomena I
Wednesday, March 14, 2018 (HH 003, **WedB3**)
Chair: *Limin Lu* (University of Waterloo)

2:00 PM **Molecular Dynamics Simulations of Liquid-liquid Phase Equilibrium of Ternary Methanol/water/hydrocarbon Mixtures** (WedB3a)
Xiaoyu Wang (Illinois Tech)

2:25 PM **Tears of Wine** (WedB3b)
Prerana Rathore, Vivek Sharma (University of Illinois at Chicago)

2:50 PM **Solvent-Dependent Self-Assembly of Biliverdin Nanoparticles for Biological Imaging** (WedB3c)
Parinaz Fathi (University of Illinois at Urbana-Champaign)

Tutorial Session: Basic Mixing and Baffling
Wednesday, March 14, 2018 (HH 010, **WedB4**)
Chair: *Reza Mostofi* (UOP / Honeywell)

2:00 PM **Basic Mixing and Baffling** (WedB4a)
Gail Pogal (SPX Flow)

YP Workshop: Mock Interviews
Wednesday, March 14, 2018 (HH 007, **WedB5**)
Chair: *Kimberly Douglas* (Abbott)
Co-Chair: *Larry Avtzis* (CB&I)

2:00 PM **Mock Interviews** (WedB5a)

Bio Based Products and Fuels
Wednesday, March 14, 2018 (HH 002, **WedC1**)
Chair: *Ignasi Palou-Rivera* (AIChE RAPID Manufacturing Institute)

3:30 PM **High Value Bioproducts--A Necessary Detour on the Road to a Robust Bioeconomy?** (WedC1a)
Mike Schultz (PTI Global Solutions)

3:55 PM **Lignin-based cell factories: Using metabolomics to guide strain engineering in Acinetobacter baylyi ADP1** (WedC1b)
Stephen Lillington, William Bothfeld, Keith Tyo (Northwestern University)

4:20 PM **Upgrading Hydrothermal Liquefaction Biocrude Oil Converted from Animal Waste** (WedC1c)
Patrick Dziura, Yuanhui Zhang, Grace Chen (University of Illinois at Urbana-Champaign) [**canceled**]

Bio-Medical Engineering III
Wednesday, March 14, 2018 (HH 005, **WedC2**)
Chair: *Parinaz Fathi* (University of Illinois at Urbana-Champaign)

3:30 PM **Defined Host–Guest Chemistry on Nanocarbon for Sustained Inhibition of Cancer** (WedC2a)
Fatemeh Ostadhossein, Santosh K. Misra (University of Illinois Urbana Champaign)

3:55 PM **Lost in Translation: Mapping the Ribosomal Active Site in Vitro** (WedC2b)
Tasfia Azim, Anne d'Aquino, Adam J. Hockenberry, Michael C. Jewett (Northwestern University), *Nikolay Aleksashin, Alexander Mankin* (University of Illinois at Chicago)

4:20 PM **Unsaturated Fatty Acid Ethyl Esters Inhibit Persister Cell Formation of Escherichia Coli and Pseudomonas Aeruginosa** (WedC2c)
Mengya Wang, Seok Hoon Hong (Illinois Tech)

Transport Phenomena II
Wednesday, March 14, 2018 (HH 003, **WedC3**)
Chair: *Caroline Szczepanski* (Northwestern University)

3:30 PM **Plowing-induced Segregation of Bidisperse Granular Mixtures** (WedC3a)
Vidushi Dwivedi, Alexander M. Fry, Paul B. Umbanhowar, Julio M. Ottino, Richard M. Lueptow (Northwestern University)

3:55 PM **Composite Membranes for Hemodialysis** (WedC3b)
Limin Lu, John Yeow (University of Waterloo)

4:20 PM **Control of Polymorphism in Continuous Crystallization** (WedC3c)
Shivani Kshirsagar, Zoltan Nagy (Purdue University)

Job Search Essentials
Wednesday, March 14, 2018 (HH 010, **WedC4**)
Chair: *Akshar Patel* (Illinois Tech)

3:30 PM **Job Searching Essentials: Utilizing Technology to Strengthen Your Job Search** (***Laptops Recommended***) (WedC4a)
Akshar Patel (Illinois Tech)

Local Section Dinner and Keynote – Ticketed Event
Wednesday, March 14, 2018 (Ballroom)
5:00 PM **Reception**
6:00 PM **Dinner**
6:45 PM **Local Section Announcements**
Janet Werner (Middough)
7:00 PM **Keynote Introduction**
Satish Parulekar (Illinois Tech)
7:10 PM **Metabolic Complexity. Is there Music Behind it?**
Doraiswami Ramkrishna (Purdue University)

AIChE Midwest Regional Conference

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AIChE Midwest Regional Conference Presentation Abstracts
March 13-14, 2018

Tuesday Morning Keynote Session

Tuesday, March 13, 2018 (HH 002)
Chair: Adam Kanyuh (UOP / Honeywell)

9:00 AM Light Hydrocarbon Conversion Chemistry Challenges in an Era of Abundant Supply of Raw Material Jim Rekoske (UOP / Honeywell)

The fracking era in the United States has created an abundant supply of cheap resources light oil, naphtha, natural gas, natural gas liquids are all available in unprecedented US supply and at relatively low cost. With this availability of supply of raw materials comes unprecedented challenges of utilizing these raw materials in the most economical fashion. Challenging questions include: What products should we make? To do so on the local, distributed scale or to aggregate and build world-scale facilities? This brief talk will focus on some solutions being proposed to meet these challenges, with a focus on the cross-disciplinary research needed to develop smart, targeted solutions.

Process Safety I

Tuesday, March 13, 2018 (HH 002, TueA1)
Chair: Robert Weber (PSRG)

10:15 AM The Sweet Smell of Ammonia Hazards (TueA1a) Nicholas Train, Sean Dee, Brenton L. Cox (Exponent)

Ammonia is a commonly used refrigerant in many different industries, including food processing facilities, cold storage warehouses, and petrochemical facilities. However, when released it can pose a serious threat to workers. Ammonia is a highly toxic chemical that is corrosive to the skin, eyes, and lungs, and at concentrations of only 300 ppm, ammonia can pose a life-threatening risk. This presentation will provide an overview of the common hazards associated with ammonia, and discuss the different ways in which ammonia spills and releases can occur. Case studies will be presented of an ammonia release caused by hydraulic shock and an ammonia release due to the rupture of a heat exchanger. These case studies will show some of the possible ways in which ammonia releases can occur, and also discuss the lessons that can be learned to mitigate these risks in the future. The case studies will also highlight the importance of responding properly to an emergency and having proper onsite emergency response training.

10:40 AM Mitigation of Flammable and Toxic Hazards through Facility Design: Beyond Code Minimums (TueA1b) Bryan Haddon, Craig Vesely (Affiliated Engineers, Inc.)

When handling flammable and toxic liquids, gases, and dusts, process facilities often must overcome numerous challenges to ensure a safe environment for their workers and neighbors. Production pressures, operational complexities, tight budgets, and an ever-changing regulatory landscape lead to challenges for the modern operating plant. By implementing engineering controls and assisting procedural controls, a facilitys design can be leveraged to mitigate many process hazards. Discussion will include Applicable Codes and Standards, implementation in a hazard analysis framework, mitigation technologies, and practical case studies.

11:05 AM PHA facilitation and How it Dovetails with Negotiation Techniques (TueA1c) Herena, Peter (Baker Risk)

Reaction Engineering

Tuesday, March 13, 2018 (HH 005, TueA2)
Chair: Mohammad Asadi (Illinois Tech)

10:15 AM Effect of Phosphate Salts and Solution pH in the Aqueous-phase Homo and Co-polymerization of NVP (TueA2a)
Fernando Borges, Fouad Teymour (Illinois Tech)

Poly(N-vinylamides), such as N-vinyl pyrrolidone (NVP), have been extensively used as monomers in the synthesis of crosslinked hydrogels, finding widespread applications in multiple industries. Our group has focused on the design and fabrication of phosphate loaded hydrogel nanoparticles copolymerized with PEGDA and NVP using inverse phase miniemulsion polymerization for applications in drug delivery, more specifically to deliver potassium monophosphate (Pi) and sodium hexametaphosphate (PPi) to the intestinal track in an effort to suppress bacterial virulence. N-vinyl pyrrolidone (NVP) aqueous-phase free-radical polymerization has been shown to decrease with increasing monomer concentration due to a solvent effect assigned to intermolecular interactions resulting in a significant hindrance of internal rotational motion in the transition state structure for propagation. We hypothesize that the addition of such salts to the NVP monomer solution could affect the interactions of the transition state structure in a way to hinder more its internal rotational motions due to the salts highly ionic nature. In this paper, we analyze the effect of two phosphate salts, potassium monophosphate (Pi) and sodium hexametaphosphate (PPi), in the aqueous-phase free-radical batch polymerization of NVP and in the copolymerization of NVP with PEGDA. Beside there is a apparent contradiction in the literature about the effect of solution pH in the polymerization kinetics. In this paper we also analyze the influence of solution pH in the aqueous-phase homo polymerization of NVP and copolymerization with PEGDA to try to answer this contradiction.

10:40 AM Imidazolinium Based Porous Hypercrosslinked Ionic Polymers for Efficient CO_2 Capture and Fixation with Epoxides (TueA2b)
Jing Li, Jiahua Zhu (University of Akron), Jun Wang, Yu Zhou (Nanjing Tech University)

The efficient capture and chemical conversion of carbon dioxide (CO_2) requires a solid simultaneously with a large surface area and highly effective active sites. Herein, imidazolinium based porous hypercrosslinked ionic polymers (HIPs) with a high surface area, rich micro/mesoporosity and abundant ionic sites were constructed via the hypercrosslinkage of 2-phenylimidazoline and benzyl halides, in which quaternization and FriedelCrafts alkylation happened simultaneously to afford ionic polymeric networks. The obtained HIPs were efficient in the selective capture of CO_2 and cycloaddition of CO_2 with epoxides. High yield, stable reusability and good substrate compatibility were achieved under mild conditions (down to ambient conditions), dramatically outperforming the homogeneous ionic liquid monomer and post-modified analogues. The synergistic adsorption and conversion enabled the efficient low-temperature conversion of diluted CO_2 (0.15 bar CO_2 and 0.85 bar nitrogen, the simulation offlue gas) catalyzed by HIPs in the presence of co-catalyst $ZnBr_2$. The in situ formed ionic sites with a high leaving ability being homogeneously embedded in the hypercrosslinked polymeric skeleton responded to the high adsorption and catalysis performance. This work highlights the functional HIPs as a versatile platform to reach efficient CO_2 capture and conversion under mild conditions.

11:05 AM Design of the Next Generation Polymerization Reactor using CFD (TueA2c)
Dimitri Gidaspow (Illinois Tech)

Two types of fluidized bed bubbling reactors are used to-day, both developed at Union Carbide in the 1970th (US Patent 3.922,322). The first built with an expanded section on top and modeled to-day using CFD suffers from severe sheet formation that forces frequent reactor shut-down.The second with internal cooling tubes is potentially better, but can be significantly improved. CFD simulations in progress (US patent, in preparation) show that a fluidized bed reactor can be constructed that solves the sheet formation problem and the low conversion which limits the polymer production rate.

Tutorial Session: Particulate Processing

Tuesday, March 13, 2018 (HH 003, TueA3)
Chair: Reza Mostofi (UOP / Honeywell)
Co-Chair: Donald Chmielewski (Illinois Tech)

10:15 AM What is s a Particle? (TueA3a) Ben Freireich (Particulate Solid Research, Inc.)

In the US, when a chemical engineering student graduates to work in the chemical process industry, there is an 80% chance their first project will involve particle technology. On average, students in the US have a cumulative 18 minutes of particle technology in their chemical engineering undergraduate curriculum. This discrepancy is particularly insidious as many concepts of solids processing are counter intuitive, and engineers feel as though they must guess. The result is significantly delayed startup ties and capacities for operations involving processing of solids. In this talk we will outline several of the most important concepts of solids processing, and show that good science in the area does exist. We will show these concepts with anecdotes from industry and some demonstrations that will probably make a mess. In the end, hopefully you will be less likely to guess.

Tuesday Plenary Session I

Tuesday, March 13, 2018 (HH 002)
Chair: Brenton L. Cox (Exponent)

12:45 PM Dust Explosion Dynamics: Combustion Theory as a Bridge to Better Safety Management Russell A. Ogle (Exponent)

A diverse range of seemingly harmless materials become explosion and fire hazards when they are transformed into finely divided, particulate matter. Any material that can be oxidized can support combustion if it is composed of sufficiently small particles. Although combustible dusts are most commonly associate with coal mines, grain elevators, and sawmills, they are found in even more hazardous forms in the plastics, petrochemical, and pharmaceutical industries.

Over the last 100 years, industrial safety experts have published a large body of empirical literature on the prevention and mitigation of combustible dust hazards. However, during this same period, combustion science has evolved into a sophisticated body of knowledge grounded in the fundamentals of thermodynamics, transport phenomena, and chemical kinetics. There is an opportunity to bridge the gap between theory practical art and fundamental science, and to place dust hazard management on a firmer, more scientific basis.

Dust explosion dynamics is the application of combustion science to better understand combustible dust hazards. Combustible dusts give rise to four basic hazard scenarios: smoldering fires, flash fires, deflagrations (explosions), and flame acceleration. This talk will illustrate how combustion science can be used to derive fundamental insights about these four hazard scenarios. Examples will be presented to illustrate the application of dust explosion dynamics to dust hazard analysis.

Tuesday Plenary Session II

Tuesday, March 13, 2018 (HH 005)
Chair: Fouad Teymour (Illinois Tech)

12:55 PM Amine-Modified Silicates as CO2 Sorbents and Catalysts Christopher W. Jones (Georgia Tech)

Worldwide energy demand is projected to grow strongly in the coming decades, with most of the growth in developing countries. Even with unprecedented growth rates in the development of renewable energy technologies such as solar, wind and bioenergy, the world will continue to rely on fossil fuels as a predominant energy source for at least the next several decades. The Intergovernmental Panel on Climate Change (IPCC) has stated that anthropogenic CO 2 has contributed measurably to climate change over the course of the last century. To this end, there is growing interest in new technologies that might allow continued use of fossil fuels without drastically increasing atmospheric CO 2 concentrations beyond currently projected levels. In this lecture, I will describe the design and synthesis, characterization and application of new aminosilica materials that we have developed as cornerstones of new technologies for the removal of CO 2 from dilute gas streams. These chemisorbents efficiently remove CO 2 from simulated flue gas streams, and the CO 2 capacities are actually enhanced by the presence of water, unlike in the case of physisorbents such as zeolites. Interestingly, the heat of adsorption for these sorbents is sufficiently high that the sorbents are also capable of capturing CO 2 from extremely dilute gas streams, such as the ambient air. Indeed, our oxide-supported amine adsorbents are quite efficient at the direct air capture of CO 2 and we will describe our investigations into development of air capture technologies as well. Finally, the amine-modified silica materials have also been used as efficient catalysts in coupling reactions important in organic synthesis, such as aldol and nitroaldol condensations. Inspired by biological catalysts that make and break bonds using cooperative organocatalytic sites, chemocatalysts designed to promote cooperativity between amines and hydrogen bonding sites are shown to be highly effective catalysts. Amine-modified silica materials present a versatile platform for diverse engineering applications.

Process Safety II

Tuesday, March 13, 2018 (HH 002, TueB1)
Chair: Brenton L. Cox (Exponent)

2:00 PM O_2 No! - Safety Considerations for Oxidation Reactions (TueB1a) Miguel E. Garcia, Brenton L. Cox, Sean Dee (Exponent)

Molecular oxygen is widely used in different chemical processes, either to produce desired chemicals by oxidation or to eliminate undesired ones. Although air is a natural source of oxygen, many oxidation reactions are improved by using an oxygen enriched mixture (concentration greater than air) or pure oxygen. Naturally, hazardous consequences arise when handling these enriched mixtures since oxygen is a component of the fire triangle and the ignition potential and oxidation rate of different substances can change dramatically in oxygen enriched atmospheres. This presentation will show case studies such as the loss of oxygen containment in an ethoxylation process and how the pressure and velocity of the oxygen stream affect the ignition potential of different components. Lessons learned from this and other cases have led to solutions on how to improve the design, operation, and maintenance of the oxidation processes, as well as the safeguards that are typically used in order to prevent accidents and mitigate the process risk.

2:25 PM Process Safety: Leading key performance indicators (TueB1b) Scott M Wozniak (UOP/Honeywell) [**canceled**]

The overall aim is to enable companies to establish effective leading indicators that proactively assess the health of barriers that manage the risk of process safety events, particularly those that could result in a major incident. A four tier model for implementation of process safety Key Performance Indicators (KPIs) and that there is a need for higher numbers of KPIs at the more leading levels. The concept of barriers is central to management of process safety risks. The bow tie and Swiss Cheese risk models are used to explained how risks can be controlled to prevent process safety events. The new revision of API 754 will also be discussed.

2:50 PM Defining "Adequate" in Adequate Ventilation (TueB1c) Matthew S. Walters, Sean Dee, Brenton L. Cox (Exponent)

Ventilation of enclosed spaces is essential in the process industry to prevent the formation of a hazardous environment due to the buildup of vapors or gases. Safety standards often specify the need for adequate ventilation, but do not provide details for what is considered adequate. This presentation will provide guidance on how to determine what constitutes an adequate ventilation rate for safe operation of a system. Methods to calculate ventilation requirements will be reviewed and their limitations examined. Two case studies will be presented: (1) maintaining the vapor space of a railcar to below the lower explosive limit (LEL) during unloading and (2) limiting the toxic gas concentration in a building that houses a chemical reactor to under the OSHA permissible exposure limit (PEL). Non-ideal mixing effects, stagnant zones, and the potential effect of buoyancy will be briefly discussed. These case studies demonstrate that while it is generally apparent when ventilation of an enclosed space is necessary, the actual air changeover rate needed for adequate venting is often non-obvious. Proper understanding of ventilation requirements can mitigate flammability and toxic hazards within enclosed spaces.

Catalysis I

Tuesday, March 13, 2018 (HH 005, TueB2)
Chair: Masoudeh Ahmadi (University of Louisville)

2:00 PM Effect of Pt, Mo, Fe, Mg and Ni Promoters on $Al_2O_3-CeO_2$ Catalyst for Oxidative Dehydrogenation of methane with Carbon Oxide (TueB2a) Abbas Jawad, Fateme Rezaei, Ali A. Rownaghi (Missouri University of Science and Technology) [**canceled**]

The promotional effect of Ni in the presence and absence of Pt, Mo, Fe and Mg were studied over Al2O3-CeO2 catalysts for the oxidative dehydrogenation of methane with carbon oxide. The reaction was conducted in a continuous fixed-bed flow reactor at 500-700 ^{o}C, space velocity of 1143 mLg-1h-1 (pure CH4 or 50% CH4 and CO2 mixture) at atmospheric pressure for 10 h time-on-stream. The catalysts were characterized by XRD, FTIR, surface area and H2-TPR analysis, and the correlation between catalyst characteristics and catalyst properties is discussed. The feed, reaction temperature, and second promoters were decisive parameters for achieving maximum methane conversion, ethene yield and CO/H2 ratio. Catalysts with imetallic promoters were more resistant toward coking.

2:25 PM Enhancing Energy Efficiency in Saccharide-HMF Conversion with Core/shell Structured Mi-

crowave Responsive Catalysts (TueB2b) Tuo Ji, Jiahua Zhu (University of Akron)

Core/shell structured microwave responsive catalysts with carbon nanotube core and active components shell were synthesized in this work for catalytic conversion of saccharide to 5-Hydroxymethylfurfural (HMF). The microstructure and surface property of these hybrid composites were carefully characterized. With such a structure of inner microwave absorber and outer catalyst shell, the heat generated at the core area by microwave radiation can be translated to the shell catalyst directly. Such localized heating allows maximum heat utilization in the reaction and uplifts the energy efficiency of the catalytic reaction. Two kinds of active components-titania and polyaniline were systematically investigated including shell thickness, surface morphology and microwave absorption efficiency towards HMF synthesis. These catalysts have been demonstrated effective in the hydrolysis conversion of various saccharides such as fructose, glucose and sucrose.

2:50 PM Electrochemistry and Structure of Doped Li_2FeSiO_4/C **Material as a Cathode for Li-ion Batteries (TueB2c)** Kamil Kucuk, Carlo U. Segre, Elena V. Timofeeva (Illinois Tech)

Rechargeable lithium ion batteries (LIBs), currently used in both electronic devices and in electric vehicles (EV), use expensive and toxic cathode materials such as layered lithium cobalt oxide ($LiCoO_2$), lithium nickel manganese oxide ($LiNi_xMn_yCo_zO_2$) mostly because of presence of Ni and Co elements.[1,2]. Among other cathode materials, polyanion compounds ($LiFePO_4$, $LiVO_3$, etc.) have also been studied as the promising LIB cathode candidates due to safety, good stability and low cost [3]. Lithium iron orthosilicate (Li_2FeSiO_4, LFS) is a member of polyanion compound family [4], with theoretical capacity of 331 $mAhg^{-1}$.[5]. The drawback of this material is its low electronic conductivity, affecting electrochemical performance. The objective of this study is to improve the electrical conductivity of LFS material through doping with tri-valent cations in Fe and Si sites as well as reducing the particle size to nanoscale and coating with conductive carbon shells. Structural, morphological and phase analysis of the family of LSF materials correlated to their electrochemical performance will be discussed, including results from x-ray diffraction, scanning electron microscopy with energy dispersive x-ray analysis, thermogravimentric analysis, FTIR and Raman spectroscopy, and electrochemical characterization (galvanostatic charge/discharge, cyclic voltammetry, impedance spectroscopy). Fe K-edge x-ray absorption spectroscopy, providing local environment of Fe atoms in pristine and doped LFS samples will also be presented.

Modeling of Bio and Pharmaceutical Processes

Tuesday, March 13, 2018 (HH 003, TueB3)
Chair: Fatemeh Ostadhossein (University of Illinois at Urbana-Champaign)

2:00 PM Agent-Based Modeling of Mammalian Cell Culture (TueB3a) Robert Jackson, Ali Cinar (Illinois Tech)

Agent-Based Modeling is a novel modeling paradigm being applied to Biological Systems. Agents are autonomously acting computational entities that sense their environment and behave based on a programmed rule-based. Chinese Hamster Ovary (CHO) Cells can naturally be represented by agents and their environment is the bioreactor media. This work shows how Agent-Based Modeling can be use to predict cell cycle phase distribution and glucose and lactate concentrations based on CHO Cell consumption and production of these nutrients/metabolites. The rule-base has been expanded to include hydrodynamic variables.

2:25 PM A Spatiotemporal Model Reveals Self-Limiting Receptor Crosslinking by Multivalent Antigens (TueB3b) Dipak Barua, Md Shahinuzzaman (Missouri University of Science and Technology)

Aggregation of cell-surface receptor proteins by multivalent antigens is an essential early step for immune cell signaling. A number of experimental and modeling studies in the past have investigated multivalent ligand-mediated aggregation of IgE receptors in the plasma membrane of mast cells. However, understanding of the mechanisms of IgE receptor aggregation remains incomplete. Experimental reports indicate that IgE receptors forms relatively small and finite-sized clusters when stimulated by a multivalent ligand. In contrast, modeling studies have shown that receptor crosslinking by a trivalent ligand may lead to the formation of large receptor superaggregates that may potentially give rise to hyperactive cellular responses. In this work, we have developed a Brownian Dynamics-based spatiotemporal model to analyze IgE receptor aggregation by a trivalent antigen. Unlike the existing models, which implemented nonspatial simulation approaches, our model explicitly accounts for the coarse-grained site-specific features of the multivalent species (molecules and complexes). The model incorporates membrane diffusion, steric collisions, and sub-nanometer-scale site-specific interaction of the time-evolving species of arbitrary structures. Using the model, we investigated temporal evolution of the species and their diffusivities. Consistent with a recent experimental report, our model predicted sharp decay in species mobility in the plasma membrane in response receptor crosslinking by a multivalent antigen. We show that, due to such decay in the species mobility, post-stimulation receptor aggregation may become self-limiting. Our analysis reveals a potential regulatory mechanism suppressing hyperactivation of immune cells in response to multivalent antigens.

2:50 PM A Study of Residence Time Distribution and Continuous Crystallization in a Dynamic Baffle Mixed-Suspension-Mixed-Product-Removal Crystallizer (TueB3c) Claire Y. Liu (Purdue University), Alastair Barton, Paul Firth (AWL), Jonathon Speed (Keit Spectrometers) [**canceled**]

The residence time distribution (RTD) is studied in the dynamic baffled crystallizer (DBC) with homogeneous and heterogeneous tracers at different mixing conditions using design of experiment (DOE) techniques. The results are then used to select an optimized operating condition for continuous crystallization. A comparison between continuous crystallization in a stirred tank and dynamic baffle crystallizer is carried out to assess the differences in final product properties. Continuous operation in both vessels is achieved using peristaltic pumps and vacuum for slurry removal. Continuous cooling crystallization of paracetamol is then evaluated in both crystallizers at the same feed concentration and mean residence time with varying power density levels. At each power density level, the start-up time and steady state crystal properties (i.e. mean size, CSD) are analyzed to determine the effect of hydrodynamics. A rigid and robust online FTIR probe, capable of correcting for signal interference caused by oscillations, is used to monitor the solute concentration during operation. This study will improve the understanding of oscillatory systems as an alternative crystallization vessel and the understanding of the impact of different mixing mechanisms on the final crystal size distribution.

Refining and Petrochemical Engineering

Tuesday, March 13, 2018 (HH 002, TueC1)
Chair: Jeffrey Zalc (BP)
Co-Chair: Hadjira Iddir (UOP/Honeywell)

3:30 PM Failures of Tubes in a Refinery Coker Furnace Due to Carburization (TueC1a) Gerald W. Wilks (CITGO Petroleum Inc.) [**canceled**]

A 9Cr-1Mo tube in the convection section of a coker furnace at Lemont Refinery failed on the morning of February 8, 2017 while this furnace was being started after being decoked with mechanical pigging. The leak resulted in a small, short duration fire inside the furnace, and the furnace was taken off line. The failed tube was replaced, and the furnace was given a hydrotest to evaluate if it was fit-for-service. During the hydrotest two more tubes failed, but these failures werent the same as the original failure. Tube samples were obtained and analysis revealed that the cause of the original failure was carburization of the ID surface of the tubes. For carburization to occur inside furnace tubes there would have had to be some source of oxygen inside the tubes because CO is needed for transport of the carbon into the steel surface. It is believed that crude composition has changed resulting in oxygen containing molecules being present inside the tubes that break down to produce CO inside the tubes. The carburization also was the root cause of the brittle tube failures that occurred during the hydrotest.

3:55 PM Fluidized Bed Stripper Hydrodynamics for Grating and Disk and Donut Trays (TueC1b) Allan S. Issangya, S.B. Reddy Karri, T. Knowlton, R. A. Cocco, B. Freireich (Particulate Solid Research, Inc.) Fluidized bed strippers are flowing fluidized beds where an up-flowing gas removes (strips out) a gaseous product entrained in a down-flowing stream of the emulsion phase. The stripper has to facilitate the transfer of the gas in the interstices of the emulsion phase and that adsorbed on the particles into the bubbles of the stripping gas. Major industrial applications of fluidized bed strippers are in fluid catalytic cracking (FCC) and fluid coking processes.

4:20 PM Simplifying Hydrogen Production (TueC1c) Alec Rockwell (Johnson Matthey)

Steam reforming based hydrogen plants involve complex and energy intensive, multi-stage operations to convert hydrocarbons into high purity hydrogen. In a complex refinery, these plants are relied on to make hydrogen for hydroprocessing units in which the hydrogen is becoming of greater value to the overall operation. The barriers to achieve this reliability are increasing for the operator. For feed purification, high level sulfur specs on natural gas pipelines, varying sulfur speciation and levels in natural gas sources, and use of high-hydrogen refinery off-gases with heavier tails can result in condition changes, spikes, and transients in operation that challenge this reliability. For the steam methane reformer (SMR), heat transfer limitations across the reformer tubes, carbon formation and poisoning, rate changes in response to hydrogen demand, and increase in pressure drop in response to shutdowns and operation also challenge this reliability. New purification and reforming technologies that deal with and remove these barriers for the hydrogen plant operator will be presented; these technologies can be implemented in existing plants with little to no capital expenditure. Experiences, support work and case studies will demonstrate how these barriers to reliability are being removed. For new plant designs, these technologies can minimize cost by removing vessels or decreasing the size of the plant, providing process simplification and intensification to hydrogen production as ever increasing demand for hydrogen and pressure on costs in the refinery make these technologies an attractive option.

Catalysis II

Tuesday, March 13, 2018 (HH 005, TueC2)
Chair: Fernando Borges (Illinois Tech)

3:30 PM Fabrication of Single Phased Iron Carbide Nanoparticles and Derived Heterostructures as Catalysts for Fischer-Tropsch Synthesis (FTS) (TueC2a) Ce Yang (Argonne National Laboratory)

Iron based FTS catalysts comprised various iron species including FeOx (Fe_2O_3, Fe_3O_4), Fe and FeC_x (Fe_5C_2, Fe_2C, Fe_7C_3, etc), which hindered the understanding of mechanism and the optimization of iron-based FTS catalysts. Among all the iron species in the catalysts, FeC_x has been long considered as the active phase of iron based FTS. However, there lacks a method to control synthesis single phase iron carbides catalysts. In a series of studies, Ce Yang et al. started with the synthesis of iron carbide (Fe_5C_2) nanoparticles by facile wet chemical route, and found that Fe_5C_2 as an active phase for FTS.[1] Then by a home-built operando characterization system, the synthetic mechanism of Fe_5C_2 was investigated, and synthesis was expanded to single phase Fe, Fe_7C_3, Fe_2C, Co_2C, $(FeCo)_5C_2$ catalysts.[2-5] By comparing the catalytic behaviors of the various iron catalysts, Fe_5C_2 was identified as the most active phase for FTS. Therefore, using Fe_5C_2 as a platform, new low-temperature iron based FTS catalysts such as Fe_5C_2/Co and Fe_5C_2/Pt was constructed by a second growth strategy.[6-7] In particular, the Fe_5C_2/Co catalysts, with only 0.6wt% Co loading, exhibits an activity similar to impregnated Co catalysts (7wt%) and four times higher than that of pure Fe_5C_2 catalyst at low temperature. Based on the mechanistic studies through temperature programmed technique, Co was responsible for the CO dissociation while

Fe_5C_2 was responsible for the chain growth at 220^{o}C. The synergistic effect of both sites lead to enhanced performance in the FTS reaction. The series of studies provides a perspective to design new FTS catalysts with desired performance based on single phased iron carbide platforms.

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3:55 PM Structural Studies of Capacity Activation and Reduced Voltage Fading in Li-Rich, Mn-Ni-Fe Composite Oxide Cathode (TueC2b) Shankar Aryal, Carlo U. Segre, Elena V. Timofeeva (Illinois Tech)

Li-rich manganese, nickel and iron (MNF) composite oxide cathodes are emerging as low cost alternative to commercial manganese nickel cobalt oxides (MNC or NMC). At cost of raw iron being three orders of magnitude lower than cobalt, MNF materials have demonstrated potential for high capacity and high discharge voltage cathodes, however, the capacity decay and instability of discharge voltage upon cycling still need to be resolved for their commercialization. Both phenomena are related to the changes in material crystal structure and in this study we utilize synchrotron x-ray diffraction (SXRD) and x-ray absorption spectroscopy (XAFS) to investigate the structural changes correlated to electrochemical performance of a representative composition of nanoscale cobalt-free, lithium and manganese rich, layered MNF oxide cathode ($Li_{1.2}Mn_{0.5}Ni_{0.2}Fe_{0.1O2}$). This material, prepared by sol gel synthesis, showed initial discharge capacity of 226 mAhg-1 (@0.1C rate) and 93% capacity retention after 100 cycles (@0.3C). Electrode materials before and after 100 charge/discharge cycles were studied with XAFS and SXRD. In discharged state Mn atoms show a shift to the lower oxidation state and an irreversible loss of oxygen near neighbors after cycling, while Ni and Fe show only minor changes in their environment. Observed 5.87% lattice expansion after cycling from SXRD pattern fitting of pristine and cycled cathode is suggested to be the cause of voltage fade.

4:20 PM Production of Functionalized Carbon from Lignocellulosic Biomass (TueC2c) Masoudeh Ahmadi (University of Louisville)

In this work, emphasis is placed on the applied methodology to convert lignocellulosic biomass to functionalized activated carbon. The final products are technically and economically viable in industrial markets such as catalysis and electro catalysis. There has been a large amount of research and interest in the conversion of biomass to carbons for various applications. However, the challenges remain both in terms of processing time scale and also with the ability to tune the resulting carbons properties. In addition, the functionalization schemes for using the resulting carbons toward catalyst schemes require additional development. The challenges in utilizing carbon supports for catalysts include uniform dispersion of active catalyst metals and metal oxide clusters and improved catalyst and support interactions. In this study, biomass were mixed with KOH solution with different impregnation ratio followed by carbonization. Textural and chemical properties for the samples were investigated by means of XRD, SEM, BET, TEM and XPS. The textural properties of carbon were found to be strongly dependent on the carbonization method and impregnation ratio. This high surface area carbons with tunable porosity, has a potential to be used as support for catalytic applications. The carbon supports were first impregnated with tetraammine platinum nitrate to produce 5%wt Pt/C. The mixture was further dried overnight at 100 ^{o}C followed by reduction to remove the ligands of the precursor and to reduce the metal to its active elemental state. Pt/C catalyst performance was evaluated by decarboxylation reaction of oleic acid. The comparison of the liquid product distribution of our catalyst with blank catalyst indicated that Pt/C catalyst has high potential to be used for this reaction.

Tissue Engineering

Tuesday, March 13, 2018 (HH 003, TueC3)
Chair: Robert Jackson (Illinois Tech)

3:30 PM Cell Growth on Microparticles for Skin Tissue Engineering (TueC3a) Sutapa Barua (Missouri University of Science and Technology)

The objective of this work is to elucidate the adhesion, proliferation, and viability of human dermal fibroblasts cells on an engineered biomaterial scaffold for skin wound healing. Skin constitutes 5.5% of the total body weight of an adult. When it is suddenly injured, it needs to be replaced quickly, especially for patients with large-area burn injury. According to the American Burn Association report, approximately 450,000 victims received medical treatment every year. Patients need healthy skins to repair the damaged tissue. Tremendous efforts have been involved in the development of viable, tissue-engineered skin substitutes. Three types of biomaterials are currently in use for dermal replacement: human allodermis or porcine dermis (Permacol), extracted bovine collagen, and nonwoven polygalactic acid scaffolds (Dermagraft and Transcyte). While natural collagen scaffolds work well, the devil is in the detail of how they are extracted, processed, and sterilized to be fit for purpose with low risk for the patient. Accordingly, the development of alternative synthetic scaffolds is a need. Among the synthetic polymers being explored for this purpose, poly-DL-lactic-co-glycolic acid (PLGA) is the US FDA approved and most widely reported. PLGA microspheres have been studied for tissue-engineering applications owing to their injectability and biocompatibility. We prepare PLGA microspheres of 200 ?m in diameter using the solvent diffusion method, in which PLGA solution in an organic phase (dichloromethane) is precipitated out in an aqueous phase. Bio-conjugation of PLL with the surface of PLGA microparticles are performed by activating carboxyl groups of PLGA and primary amine groups from poly-l-lysine (PLL), forming amide bonds. The resulting PLL conjugated PLGA microparticles formulations are sterilized using Amicons gravity ultrafiltration. Human dermal fibroblasts are grown on PLL conjugated PLGA microparticles in liquid suspension in vitro. After 3 days in culture, the cells show high cell viability with minimal/ no cytotoxicity as quantified by the live/dead assay, flow cytometry, and fluorescence microscopy. The cells show characteristic cytoskeleton proteins after being grown on the microparticles as determined by an immunofluorescence assay. The data provide us confidence in our ability to synthesize biocompatible microparticles on which fibroblasts can attach and can be tested for implantation into the dermal wound site.

3:55 PM 3D Simulation of Bone Regeneration using Repast HPC: Optimal Scaffold Design for Bone Tissue engineering applications (TueC3b) Chenlin Lu, Mustafa C. Ozturk, Sami Somo, Eric M.Brey, Ali Cinar (Illinois Tech), Banu Akar (Northwestern University)

Bone tissue engineering (BTE) has emerged over the past few decades as a potential alternative to the field of conventional bone regenerative medicine due to the exceedingly high demand of adequate bone grafts. Regeneration of bone tissue in BTE requires synergistic combination of biomaterial scaffolds, growth factors, and osteogenic cells. Scaffolds with well-designed architectures and degradation characteristics, provided with appropriate angiogenic and osteogenic factors are essential for bone tissue regeneration. Taking into account these factors that contribute to bone tissue regeneration process simultaneously and optimizing their characteristics presents a highly difficult task and cannot be addressed with experimentation alone. Computational models combined with experimental methods provide us better understanding of the underlying mechanisms of the complex process. This understanding is critical for the design of various parameters which can lead to optimized bone tissue regeneration. Agent-based modeling (ABM) is a powerful modeling and simulation technique and is naturally suitable for complex biological system as it simulates actions and interactions of individual agents in an attempt to re-create and predict the appearance of complex phenomena. Repast HPC toolkit, an ABM tool for high-performance computing environments, is utilized to simulate engineered bone tissue growth in a porous biomaterial scaffold. 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 [2,3], were combined together to investigate the comprehensive process. Using the baseline Repast HPC tools provides flexibility for continued model development and improvement. The simulation results indicate that scaffold architecture and growth factors play an important role in bone tissue regeneration. Simulations show the flexibility of the developed ABM and exemplify the types of investigation it enables. These results can combine with experimental data to help us design optimal biomaterial scaffolds for bone tissue regeneration.

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4:20 PM Personalized Absorbable Gastrointestinal Stents for Intestinal Fistulae and Perforations (TueC3c) Parinaz Fathi, Fatemeh Ostadhossein, Indu Tripathi,, Santosh K. Misra, Dipanjan Pan (University of Illinois at Urbana-Champaign), Blair Rowitz (Carle Foundation Hospital)

Gastrointestinal (GI) tract perforations are relatively frequent surgical emergencies, are potentially life-threatening, and can occur from several different sources. In general, treatment requires urgent surgical repair or resection and at times can lead to further complications. Currently available stents are non-absorbable, are manufactured in a narrow size range, and/or are limited to usage in locations that are accessible for endoscopic removal post-healing. The use of 3D-printed bioresorbable polymeric stents will provide patients with a stent that is tailored specifically to their geometry, will degrade with time to eliminate the need for further surgeries for stent removal post-healing, and will be usable in locations that are not endoscopically accessible. This project focuses on the characterization of polycaprolactone-polydioxanone (PCL-PDO) composites for use in a bioresorbable gastrointestinal stent. Dynamic Mechanical Analysis (DMA) tests were conducted to separately analyze the effects of composition, the filament formation process, and physiological temperature on the PCL-PDO material properties. The proposed stent design was then modelled using computer-aided design, and Finite Element Analysis (FEA) was used to simulate the effects of physiologically relevant forces on stent integrity. In-vitro studies were used to evaluate the biocompatibility of the polymer composite. PCL-PDO stents were then 3D-printed and placed in-vivo in a pig model, and histological evaluation was used to determine the safety of these stents.

Wednesday Morning Keynote Session

Wednesday, March 14, 2018 (HH 002)
Chair: Ali Cinar (Illinois Tech)

9:00 AM Microfluidic Systems for the Skin John A. Rodgers (Northwestern University)

Process Engineering

Wednesday, March 14, 2018 (HH 002, WedA1)
Chair: Juan Garcia (Argonne National Laboratory)

10:15 AM Introduction to the RAPID Manufacturing Institute, Program Roadmapping and First Projects (WedA1a) Ignasi Palou-Rivera (AIChE RAPID Manufacturing Institute)

In December, 2016, the Department of Energy announced the establishment of the 10th Manufacturing USA Institute, representing a critical step in the federal governments effort to double U.S. energy productivity by 2030. The Rapid Advancement in Process Intensification Deployment (RAPID) Institute is focused on addressing the barriers listed above to enable the development of breakthrough technologies to boost energy productivity and energy efficiency through manufacturing processes in industries such oil and gas, pulp and paper and various domestic chemical manufacturers. RAPID will leverage approaches to modular chemical process intensification (MCPI) such as combining multiple process steps such as mixing, reaction, and separation into single more complex and intensified processes with the goal of improving productivity and efficiency, cutting operating costs, and reducing waste. RAPID has highlighted six focus areas to organize the scope of research and development activities in the institute. These include 3 application areas that were selected based on the high level of energy/capital intensity or their potential to benefit from widely distributed modular technologies:
1) Chemical & Commodity Processing
2) Natural Gas Upgrading
3) Renewable Bioproducts
Three additional areas were selected that focus on the underpinning science and technology that will be required for broader utilization of MCPI technologies
4) Modeling and Simulation
5) Intensified Process Fundamentals
6) Module Manufacturing

10:40 AM Bring it All Back to Nature: A New Paradigm in Environment-Energy-Nutrient Nexus (WedA1b) Meltem Urgun-Demirtas (Argonne National Laboratory)

There is tremendous biomass and organic waste generation in the U.S. (500 million tons of wet organic waste per year). Anaerobic digestion is a widespread proven technology adopted by U.S. wastewater treatment plants, farms, and food waste processors for waste stabilization and biogas production. Biogas is a renewable energy source with great potential to reduce dependence on fossil energy and decrease greenhouse gas emissions. However, biogas industry suffers from low productivity and high biogas upgrading and treatment cost which are the key barriers to the application of anaerobic digestion technologies in the US.

Argonne addressed these challenges by developing a patent-pending low-cost process that enhances the heating value of biogas, delivering a gas that is close to pipeline quality (greater than 90% methane) (U.S. Patent Application No. 14/540,393). Most remarkably, the treatment captures and sequesters the carbon dioxide and hydrogen sulfide that is naturally produced during biological methane production. This process also accelerates renewable methane production rates by at least 10-30% while sequestering carbon dioxide. Pilot-scale field trials were conducted in a 500-gallon mesophilic AD digester complex at Ruckman Farm facility in northern Missouri. The process is configured with a two-stage batch system with parallel second stage reactors. Pilot-scale results showed that the in situ biogas production and upgrading process is highly adaptable and scalable and enables the conversion of manure into biogas with high methane content (86%) and digestate (i.e. left over after anaerobic digestion of organic waste) with high fertilizer value, rich in macro and micro nutrients necessary for growth of crops.

11:05 AM Design of Smart Grid Responsive Energy Storage Systems (WedA1c) Oluwasanmi Adeodu, Donald Chmielewski (Illinois Tech)

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. Previously, we have demonstrated that Economic Model Predictive Control (EMPC) can be used to approximate the scenario based multi-stage stochastic programming version of the economic dispatch problem. However, since operation of storage units is expected to be at a larger time scale, it is more appropriate to consider a Unit Commitment (UC) type framework. Within this framework the multi-stage, stochastic program will contain mixed integer variables, accentuating the need for a more computationally attractive operating policy. In this work, the head-to-head comparison between EMPC and the scenario based solution is extended to the UC framework in an effort to validate the adoption of more tractable EMPC-based methods for the optimal sizing and placement of storage units.

Bio-Medical Engineering I

Wednesday, March 14, 2018 (HH 005, WedA2)
Chair: Dipak Barua (Missouri University of Science and Technology)

10:15 AM Nanosalina: A Tale of Saline-Loving Algae from the Lake's Agony to Cancer Therapy (WedA2a) Fatemeh Ostadhossein, Dipanjan Pan, Santosh Misra (University of Illinois Urbana Champaign)

The nanoparticles (NPs) that contain the therapeutic agent within themselves without further modifications can be coined as self-therapeutic NPs. The development of these agents especially when derived from natural resources can lead to a paradigm shift in the field of cancer nanotechnology as they can immensely facilitate the complex chemistry procedures and the follow up biological complications. Herein, we demonstrate that inherently therapeutic NPs integrating β-carotene can be synthesized from Dunaliella salina microalgae in a single step without complicated chemistry. The facile synthesis involved microwave irradiation of aqueous suspension of algae which resulted in water dispersible NPs with hydrodynamic diameter of 80 nm. Subsequently, extensive physiochemical characterizations were performed to confirm the integrity of the particles. The pro-oxidant activities of the integrated -carotene were triggered by photoexcitation under UV lamp (362 nm). It was demonstrated that after UV exposure, the C32 human melanoma cells incubated with NPs experienced extensive cell death as opposed to nonilluminated samples. Further cellular analysis revealed that the significant reactive oxygen species (ROS) and in particular singlet oxygen were responsible for the cells damage while the mode of cell death was dominated by apoptosis. Moreover, detailed endocytic inhibition studies specified that UV exposure affected NPs cellular uptake mechanism. These inherently therapeutic NPs can open new avenues for melanoma cancer treatment via ROS generation in vitro.

10:40 AM Cancer Cells as Signaling Factories (WedA2b) Mi Zhang, Harihara Baskaran, Roshini Balan, Reed Momjian (Case Western Reserve University)

In this investigation, we studied the effect of human breast cancer cells on their ability to induce migration of human endothelial cells in an in vitro model. First, we developed a 3-D cellular spheroid model of the cancer cells in a co-culture model with human fibroblasts and endothelial cells. We demonstrate the optimization and stability of the spheroids as a function of individual cell composition. Next, we developed a migration model in a collagen gel system and investigated the migration of the endothelial cells. Our results showed that the endothelial cell migration is greatly enhanced by the presence of cancer cells. We also present results from a mathematical model of the above system that can distinguish paracrine signaling mechanisms of cell migration.

11:05 AM Colicin Production using Cell-free Protein Synthesis to Control Persister Cell Formation (WedA2c) Xing Jin, Seok Hoon Hong (Illinois Tech)

Persister cells are metabolically dormant bacterial populations that are frequently found in biofilms and increased under environmental stresses. Since persister cells are not growing, they can survive under very high concentrations of conventional antibiotics that can kill actively growing cells, which has been a serious problem in treating chronic bacterial infections. Therefore, there is an urgent and growing need for developing novel antimicrobial drugs that can kill non-growing persister cells. Colicins, a type of antimicrobial bacteriocins, are considered as a viable alternative of conventional antibiotics due to their unique cell killing mechanisms that can damage cells by pore-forming on the cell membrane, nuclease activity, and cell wall synthesis inhibition. Additionally, colicins cell killing activity is target-specific by recognizing receptors of the target cells without influencing other bacteria. However, colicin production requires co-production of immunity protein to protect host cells, otherwise the colicins are lethal to the host. To maximize the colicin production and avoid the cell viability concerns without co-production of immunity protein, we utilized cell-free protein synthesis to produce colicins with different modes of action. Cell free synthesized colicin M (peptidoglycan inhibitor), Ia (pore-forming), E1 (pore-forming), and E2 (nuclease) killed the actively growing cells of Escherhichia coli in a nutrient-rich medium. However, when tested the cytotoxicity of colicins in a nutrient-free medium, only colicins E1 and E2 exhibited efficient killing of non-growing cells. Then, we examined to see if colicins can kill persister cells upon antibiotics treatment. Colicin E1 and E2 effectively killed persister cells prepared from both exponential as well as stationary phase cells by treating with Ciprofloxacin antibiotic. This study supports that colicins can be developed to kill persister cells that are responsible for chronic diseases, and cell-free protein synthesis can be used as a promising platform for rapid production and characterization of toxic proteins.

Bio-Interfaces

Wednesday, March 14, 2018 (HH 003, WedA3)
Chair: Yongbeom Seo (University of Illinois at Urbana-Champaign)

10:15 AM Probiotic Escherichia Coli Outcompetes Pathogens during Biofilm Formation (WedA3a) Kuili Fang, Seok Hoon Hong (Illinois Tech), Shweta Shree (Birla Institute of Technology)

Biofilms are sessile microbial communities formed on the biotic and abiotic surfaces by the secretion of extracellular polymeric substances that enhance adherence to the surfaces and microbial aggregation. Biofilm bacteria are highly tolerant to exogenous stresses such as antibacterial agents due to mass transfer limitation in biofilm matrix and non-metabolizing nature of cells inside the biofilms. Many pathogens take advantages of living as biofilms, and thus 75% of human infectious diseases is closely involved in the formation of biofilms. Therefore, understanding the biofilm formation is critical to establishing novel strategies of controlling infectious diseases. Although the majority of biofilm studies has examined mono-species cultures, the biofilm formation is intra- and inter-species phenomena that require dynamic interactions between bacteria in mixed biofilm communities. However, little is known to understand molecular interactions between biofilm bacteria. Escherichia coli strain Nissle 1917 (EcN) is a probiotic bacterium that has antagonistic effects on adherence, growth, and biofilm formation of other E. coli strains. In this study, we investigated the ability of EcN to outcompete with the biofilm formation of pathogenic bacteria such as pathogenic E. coli (EHEC), Pseudomonas aeruginosa, Staphylococcus aureus, and S. epidermidis. In dual-species biofilms, EcN repressed biofilm formations of EHEC, S. aureus, and S. epidermidis while it did not inhibit biofilms of P. aeruginosa. As a control, commensal E. coli did not reduce the biofilm formation of pathogenic bacteria. We identified from mass spectrometry analysis that DegP known as a protease of EcN is responsible for inhibiting EHEC biofilms. In addition, through transposon mutagenesis screening of EcN, we identified four mutants that are involved in repressing biofilms of EHEC as well as two Staphylococcus species. These results provide insights in applying and developing probiotics as an effective treatment for the biofilm-related infectious diseases.

10:40 AM Photopolymerization Techniques to Design Biomimetic, Micro-structured Interfaces (WedA3b) Caroline Szczepanski (Northwestern University)

Over time, nature has provided countless examples of surfaces with unique interfacial behaviors. From the lotus leaf, which strongly repels water, to the Namib desert beetles shell, which permits these creatures to attract and collect water necessary for survival in the most arid of climates, there are numerous examples of interfaces with unique or unexpected behaviors. These interfacial phenomena are incredibly useful for engineering applications such as designing coatings to protect structures, developing devices that aid with the capture and retention of water in harsh environments, etc. Through observations of varied natural surfaces, such as the lotus leaf, it has been established that both surface chemistry as well as topological features ranging in scale from nanometer to micron play a significant roles in interfacial interactions. With these combined influences, it is necessary to identify versatile and efficient methods to develop surfaces where both control over surface chemistry and topography are afforded. In this talk, we will explore the use of photopolymerization-based approaches to engineer surfaces with features and behavior similar to natural interfaces, addressing the need for both topological features and chemical patterning. Photopolymerizations are attractive to address this engineering challenge, since photo-based fabrication techniques offer both spatial and temporal control. Furthermore, the use of photopolymerizations is an energy efficient approach to polymer design and fabrication, particularly when compared to thermal-based processes. I will highlight how photopolymerization parameters (e.g. irradiation intensity) can be used to manipulate the surface chemistry and chemical patterning of interfaces composed of copolymer resins, by altering thermodynamically driven de-mixing across a surface. Furthermore, I will show how our recent work indicates that polymerization-induced shrinkage can be exploited to create surface patterns, addressing the need for topological features in addition to chemical patterning. I will highlight how these topological features can be manipulated by considering coating / substrate interactions. Lastly, I will show how these combined influences can be used to rapidly develop a surface that mimics the morphology and wetting behavior of rose petals.

11:05 AM Temperature-dependent Synthesis of Multicolored Carbon Dots with Inherent Surface-Abundant Functionalities (WedA3c) Parinaz Fathi, Indrajit Srivastava, Santosh K. Misra, Dipanjan Pan (University of Illinois at Urbana-Champaign)

Carbon dots have garnered attention for their interesting fluorescent properties and their biocompatibility, which make them ideal for applications in biological imaging and drug delivery. Specifically, carbon dots with emission in the yellow or further red-shifted wavelengths provide a promising platform for biological imaging with minimal interference from blood and tissue autofluorescence. Here we present the synthesis and characterization of multicolored inherently functionalized carbon dots from a variety of carbon sources and at multiple synthesis temperatures. The carbon dots were characterized using transmission electron microscopy (TEM), UV-Vis spectroscopy, fluorescence spectroscopy, fluorescence imaging, Fourier Transform Infrared Spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS). We found that functionalized carbon dots could be obtained through a single-step synthesis method, and that small changes in synthesis temperature led to detectable red-shifting or blue-shifting of nanoparticle fluorescence. Additionally, the direction of fluorescence change based on temperature was found to vary between carbon sources. These results suggest the potential for synthesis temperature to be utilized as a simple tool for modulating carbon dot fluorescence.

Wednesday Plenary Session I

Wednesday, March 14, 2018 (HH 002)
Chair: Mike Schultz (PTI Global Solutions)

12:45 PM Future Scenarios for Renewable Transportation Fuels in a Rapidly Changing Transportation Industry Thomas Foust (National Bioenergy Center, NREL)

Wednesday Plenary Session II

Wednesday, March 14, 2018 (HH 005)
Chair: Amid Khodadoust (University of Illinois at Chicago)

12:45 PM Unexpected Behavior of Photoactive Nanocomposites in Energy Environmental Applications Kimberly Gray (Northwestern University)

Experimental and computational studies have shown that the high reactivity of the simplest TiO 2 nanocomposite (mixed phase materials) is explained by interfacial defect sites that create catalytic hot spots. This basic understanding has directed the design and synthesis of nanostructured TiO 2

-based photocatalysts for use in a variety of energy, health and environmental systems and yielded some surprising results. This presentation will review four examples that describe our efforts to drive the conversion of CO 2 to high value products, create transparent films to produce antibacterial surfaces and finally, probe the interactions of nanomaterial mixtures under environmental conditions to determine potentially toxic effects.

Electro-chemical Engineering

Wednesday, March 14, 2018 (HH 002, WedB1)
Chair: Hakim Iddir (Argonne National Laboratory)

2:00 PM Lattice Templating and Galvanic Coupling Effects on the Electrochemical Performance of Core/shell Battery Materials (WedB1a) Elahe Moazzen, Elena Timofeeva, Carlo Segre (Illinois Tech)

β-Ni(OH)2 is commonly used as the cathodic material in rechargeable aqueous battery systems due to its well-defined electrochemical redox activity, high electric potential, high theoretical specific capacity (289 mAh/g) and relatively low cost. However, β-Ni(OH)2/β-NiOOH cathodes are also known to have inherently low electrical conductivity, which often results in incomplete discharge, low Coulombic efficiency and slow rates of charge and especially discharge. In this study, Ni(OH)2 nanoparticles (100x20 nm platelets) were synthesized and coated with epitaxial Co(OH)2 shells and a series of Ni(OH)2/Co(OH)2 core/shell nanoplatelets with varying shell thickness (0.5 to 4.1 nm) were systematically investigated with a combination of scanning electron microscopy (SEM) with energy dispersive x-ray analysis (EDX), x-ray diffraction (XRD), in situ and ex situ x-ray absorption fine structure spectroscopy (XAFS), and electrochemical tests. Structure-property correlations revealed that electrochemical behavior and reversibility of Co(OH)2 redox conversion depends non-linearly on the shell thickness, with the best performance (99.6% of theoretical capacity of the composite material, 10% improvement over the performance of pristine Ni(OH)2 nanoparticles) achieved at shell thickness of 1.90.3 nm. We suggest that in addition to the improvement in electrical conductivity, such thickness dependent Co(OH)2 shell behavior and the superior performance are due to a lattice templating effect, and the galvanic coupling of core and shell materials. Homogeneous deposition of the shell is confirmed with XRD, SEM and EDX, while lattice templating effect was suggested from XAFS results showing that Co-M and Co-O distances are close to those of the Ni(OH)2 lattice in thin shells and shift gradually towards values of bulk Co(OH)2 as the shell thickness increases. From a combination of electrochemical and structural characterization of these composite nanomaterials, including in situ XAFS, galvanic coupling between the shell and core is proposed as a material activation mechanism, which explains the limited reversibility of the Co(II)/Co(III) oxidation in some cases. The prospect of applying this nanostructuring to other combinations of materials such as MnO2/Fe2O3 and Fe2O3/MnO2 will also be discussed.

2:25 PM Transition Metal Segregation and Phase Transformations on the Surfaces of Layered $Li(Ni_{1-x-y}Mn_xCo_y)O_2$ (NMC) Cathode Materials for Li-ion Batteries (WedB1b) Juan Garcia, Javier Bareno, Jason Croy, Hakim Iddir (Argonne National Laboratory), Guoying Chen (Lawrence Berkeley National Laboratory)

Layered $Li(Ni_{1-x-y}Mn_xCo_y)O_2$ (NMC) oxides are promising cathode materials capable of addressing some of the challenges associated with next-generation energy storage devices. In particular, improved energy densities, longer cycle-life, and improved safety characteristics with respect to current technologies are needed. However, transformations taking place in the positive electrodes of battery cells decrease electrochemical performance. For instance, the segregation of transition metals from the bulk to the surface of cathode particles plays a critical role in the formation of surface reconstruction layers (SRLs). Such layers are thought to decrease the performance of batteries by, for example, impeding the diffusion of lithium during charge and discharge. A preferential segregation of Ni and Co to specific facets of as-prepared, pristine NMC materials has been found previously. This presentation will discuss recent results of a computational analysis of segregation and phase transformation processes using Density Functional Theory (DFT). A discussion on the thermodynamics that govern such processes will be given.

2:50 PM In Situ EXAFS-derived Reversible Capacity Mechanisms in Sn-based Graphite Composite Anodes (WedB1c) Yujia Ding, Elena V. Timofeeva, Carlo U. Segre (Illinois Tech)

Sn-based conversion-type anode materials such as SnO_2, SnS_2 and Sn_4P_3 exhibit large theoretical capacities are the promising alternatives of traditional graphite anodes for Li-ion batteries. During the lithiation process, these materials undergo a possibly reversible conversion reaction to form metallic Sn, and followed by a highly reversible alloying reaction with Li-ions. Previous studies show that significant capacity enhancement can be achieved by introducing graphite matrix by a high-energy ball milling process. The uniformly distributed nanoscale active materials in graphite matrix enable the reversible conversion reaction in the materials by increasing electrical conductivity and preventing aggregation of Sn clusters during cycling. The detailed local structural changes correlated to their electrochemistry are studied by in situ extended x-ray absorption fine structure (EXAFS). The mechanisms of reversibility, capacity fading, and improved performance of the graphite composite materials are discussed.

Bio-Medical Engineering II

Wednesday, March 14, 2018 (HH 005, WedB2)
Chair: Sutapa Barua (Missouri University of Science and Technology)

2:00 PM Engineering Bioactive Hydrogels for Cardiac Repair (WedB2a) Arghya Paul (University of Kansas)

The objective of this project was to develop an injectable and biocompatible hydrogel that can deliver a cocktail of therapeutic biomolecules (secretome) secreted by human adipose-derived stem cells (hASCs) to the peri-infarct myocardium. Gelatin and Laponite were combined to formulate a shear-thinning, nanocomposite hydrogel (nSi Gel) as an injectable carrier of secretome (nSi Gel+). The growth factor composition and the pro-angiogenic activity of the secretome were tested in vitro by evaluating the proliferation, migration and tube formation of human umbilical endothelial cells. The therapeutic efficacy of the nSi Gel+ system was then investigated in vivo in rats by intramyocardial injection into the peri-infarct region. Subsequently, the inflammatory response, angiogenesis, scar formation, and heart function were assessed. Biocompatibility of the developed nSi Gel was confirmed by quantitative PCR and immunohistochemical tests which showed no significant differences in the level of inflammatory genes, microRNAs, and cell marker expression compared to the untreated control group. In addition, the only group that showed a significant increase in capillary density, reduction in scar area and improved cardiac function was treated with the nSi Gel+. Our in vitro and in vivo findings demonstrate the potential of this new secretome-loaded hydrogel as an alternative strategy to treat myocardial infarction.

2:25 PM Agent-Based Modeling of the interactions between lymphocytes and Beta cells in Type 1 Diabetes (WedB2b) Qian Xu, Mustafa Cagdas Ozturk,Ali Cinar (Illinois Tech)

Diabetes is one of the prevalent diseases in the USA. This work is focused on the development of a high-performance agent-based model simulating the pathogenesis of Type 1 diabetes mellitus in pancreas. Lymphocytes, such as CD8 T cells, destructive CD4 T cells, Antigen Presenting Cells and regulatory T cells are incorporated in both pancreatic lymph node and pancreatic tissue compartments. Regulatory T cells inhibit destructive T cells through direct and indirect ways. Antigen presenting cells play important but not complete role in T cell tolerance. Simulations based on models are helpful in studying the effects of changes in various variables and parameters, and can be used to formulate hypotheses to be tested experimentally. Simulations can determine the most promising ranges of the variables to influence a desirable outcome. Hence, they can reduce the cost of clinical experiments and accelerate the discovery and improvement of new therapies for diabetes. The model can capture the trends of different cell variations during the disease progression and portrays the role of different factors in the process. It is expected that, with the addition of other immune pathway and 3D model building, the model will be a valuable tool for the planning of clinical studies.

2:50 PM Active Antioxidizing Polymeric Particles for On-demand Pressure-driven Molecular Release (WedB2c) Yongbeom Seo, Hyunjoon Kong (University of Illinois at Urbana-Champaign)

Overproduced reactive oxygen species (ROS) are closely related to various health problems including inflammation, infection, and cancer. The abnormally high ROS level can cause serious oxidative damage to biomolecules, cells, and, tissues. A series of nano- or micro-sized particles has been developed to reduce the oxidative stress level by delivering antioxidant drugs. However, most systems are often plagued by the slow molecular discharge driven by diffusion. In this work, we demonstrate an active antioxidizing polymeric particles that can increase the internal pressure in response to the abnormal ROS level and thus actively discharge antioxidants to protect cells and tissues from the oxidative damage. The on-demand pressurized particles particle was assembled by simultaneously loading water-dispersible manganese oxide (MnO_2) nanosheets and green tea-derived antioxidant into poly(lactic-co-glycolic acid) (PLGA) spherical shell. In the presence of H_2O_2, one of the ROS, MnO_2 nanosheets in the PLGA particle generated oxygen gas by decomposing H_2O_2 and increased the internal pressure. Accordingly, the active antioxidizing particle system could release a larger fraction of antioxidants and effectively protect endothelial cells and brain tissues from H_2O_2-induced oxidative damage. We believe that this study would significantly impact current design paradigm of the controlled molecular releasing system and subsequently improve the efficacy of a broad array of molecular cargos.

Transport Phenomena I

Wednesday, March 14, 2018 (HH 003, WedB3)
Chair: Limin Lu (University of Waterloo)

2:00 PM Molecular Dynamics Simulations of Liquid-liquid Phase Equilibrium of Ternary Methanol/water/hydrocarbon Mixtures (WedB3a) Xiaoyu Wang (Illinois Tech)

We report molecular simulation studies of liquid-liquid equilibria (LLE) in mixtures that include polar (water/methanol) and non-polar/weakly polar (cyclic) components. While vapor-liquid equilibria (VLE) has been widely studied using molecular simulations, there have been relatively few such studies for LLE despite their industrial importance. Often equation of state parameters that work for VLE do not work well for LLE, our studies show, however, that molecular potentials for VLE were successful in predicting reliable results for LLE. Our methodology is an extension of our previous studies for VLE (solubility of gases in liquids). In these studies, we used the generalized AMBER force field (GAFF) with no further adjustments. Our results showed good agreement with recent experimental results for LLE of these systems and showed some interesting trends. We found that the behavior of mixtures of hydrocarbons with both methanol and water present became significantly different when no water was present. After validating our method and models in our LLE studies, we also used these simulations to explore other dynamic and equilibrium properties of these mixtures. Our results showed significant changes in the structural and dynamic behavior of these mixtures as the concentration of water changed.

2:25 PM Tears of Wine (WedB3b) Prerana Rathore, Vivek Sharma (University of Illinois at Chicago)

'Tears of wine' refer to the rows of wine-drops that spontaneously emerge within a glass of strong wine. Evaporation-driven Marangoni flows near the meniscus of water-alcohol mixtures drive liquid upward forming a thin liquid film, and a rim or ridge forms near the moving contact line. Eventually the rim undergoes an instability forming drops, that roll back into bulk reservoir forming so called tears or legs of wine. Most studies in literature argue the evaporation of more volatile, lower surface tension component (alcohol) results in a concentration-dependent surface tension gradient that drives the climbing flow within the thin film. Though it is well-known that evaporative cooling can create temperature gradients that could provide additional contribution to the climbing flows, the role of thermocapillary flows is less well-understood. Furthermore, the patterns, flows and instabilities that occur near the rim, and determine the size and periodicity of tears, are not well-studied. Using experiments and theory, we visualize and analyze the formation and growth of tears of wine. The sliding drops, released from the rim towards the bulk reservoir, show oscillations and a cascade of fascinating flows that are analyzed for the first time.

2:50 PM Solvent-Dependent Self-Assembly of Biliverdin Nanoparticles for Biological Imaging (WedB3c) Parinaz Fathi (University of Illinois at Urbana-Champaign)

Biliverdin is a naturally-occurring pigment in bile that exhibits high UV-Vis absorbance in the near-IR region, providing a potential platform for photoacoustic imaging with minimal background interference from biological tissue. Biliverdin nanoparticles (BVNPs) were synthesized in a variety of solvents, and were characterized using transmission electron microscopy (TEM), UV-Vis spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy / Energy Dispersive X-Ray Spectroscopy (SEM/EDS), zeta potential measurements, fluorescence spectroscopy, fluorescence imaging, and photoacoustic imaging. The nanoparticles exhibited high absorbance at 365 nm and 680 nm, fluorescence when excited at 365 nm, and photoacoustic properties when excited at 680 nm. Nanoparticles were shown to form as early as ten minutes into the synthesis, and their properties varied based on the synthesis solvent. Nanoparticles synthesized in water and 0.9% NaCl solution were found to exhibit higher absorbance and lower fluorescence compared to the nanoparticles synthesized in MES. Additionally, nanoparticles synthesized in MES exhibited a red-shifted fluorescence over time compared to the other nanoparticles. The potential of these nanoparticles for use as photoacoustic agents in lymph node imaging was demonstrated in nude mice.

Tutorial Session: Basic Mixing and Baffling

Wednesday, March 14, 2018 (HH 010, WedB4)
Chair: Reza Mostofi (UOP/Honeywell)

2:00 PM Basic Mixing and Baffling (WedB4a) Gail Pogal (SPX Flow)

This brief talk introduces the basic concepts of mixer sizing and selection. Topics include: Agitator selection for blending liquids, suspending solids in liquids or gas-liquid contacting; Differences between mixing in batch and continuous operations; Evaluating options using computational fluid dynamics (CFD) and scale modeling; Effective baffling and coordination of baffles with coils or other heat transfer surfaces is discussed; Mechanics of agitator design; Practical suggestions for specifying mixers in dynamic conditions. Gail Pogal is a Senior Applications Engineer at SPX Flow US LLC (Lightnin and Plenty Mixers). Gail holds a B.S. in Chemical Engineering from the University of Rochester and an Executive M.B.A. from the Simon Business School at the University of Rochester. She is the author or coauthor of five technical papers regarding mixing, process automation and optimization. Her areas of mixing expertise include chemical processing, pulp and paper production and gas-liquid reactions. She is a 25+ year member of AIChE and a former Chair of the AIChE- Rochester Section.

Bio Based Products and Fuels

Wednesday, March 14, 2018 (HH 002, WedC1)
Chair: Ignasi Palou-Rivera (AIChE RAPID Manufacturing Institute)

3:30 PM High Value Bioproducts–A Necessary Detour on the Road to a Robust Bioeconomy? (WedC1a) Mike Schultz (PTI Global Solutions)

Broad deployment of technologies for renewable fuel and commodity chemicals has been slowed by scaleup and implementation challenges, often driven by poor economics. An emerging trend sees startups and existing companies in the renewable/bio space shifting toward higher value products, including flavors and fragrances, proteins for fish, animals, and humans, and high value, low market specialty chemicals. While the products are quite different from fuels and commodity chemicals, the underlying technology for these higher value products is similar in many ways. This may be a temporary, but necessary, detour on the road to a robust economy that enables value creation while technical challenges in scale-up are addressed. As the industry collectively progresses in scale the technical developments for these small scale, high value products can be leveraged to improve the technologies to make biofuels and commodity chemicals, creating value in larger markets and reducing greenhouse gases at a meaningful level.

3:55 PM Lignin-based cell factories: Using metabolomics to guide strain engineering in Acinetobacter baylyi ADP1 (WedC1b) Stephen Lillington, William Bothfeld, Keith Tyo (Northwestern University)

Rapid depletion of fossil resources and an increasing threat of anthropogenic climate change are driving a need for renewable alternatives to petrochemicals. Lignin, a common waste product from paper and agriculture industries, offers a rich diversity of aromatic molecules that can be converted into biorenewable alternatives to petrochemicals. Acinetobacter baylyi ADP1 (referred to as ADP1) is an attractive candidate for lignin valorization due to its ability to metabolize a diverse array of lignin monomers and its natural propensity to incorporate foreign DNA into its genome. However, progress in engineering ADP1 for this end-use is hindered by a lack of understanding of metabolism. This hindrance is not limited to ADP1 metabolic engineering efforts in all organisms are met with a similar challenge, in which changes to the genotype often yield unpredicted changes in cellular behavior. Metabolomics, a technique that measures concentrations of hundreds of metabolites inside cells simultaneously, has the potential to fill this gap in understanding by measuring directly the metabolic signature that is most closely tied to cellular phenotype. The presented work investigates how both genetic and environmental perturbations alter metabolism in ADP1 using metabolomics. Of particular interest is the metabolic response to aromatic compounds which are concentrated in lignin hydrolysate, yet toxic to lignin-metabolizing bacteria such as ADP1 at relatively low levels. Metabolomics, combined with analytical methods for measuring protein expression and lipid membrane composition, will help elucidate mechanisms of toxicity for these aromatic compounds, as well as mechanisms that confer tolerance in ADP1. This knowledge may then be applied to engineer tolerance phenotypes in ADP1 and improve its ability to produce valuable chemical products from waste lignin.

4:20 PM Upgrading Hydrothermal Liquefaction Biocrude Oil Converted from Animal Waste (WedC1c) Patrick Dziura, Yuanhui Zhang, Grace Chen (University of Illinois at Urbana-Champaign)[**canceled**]

This study showed the implications of using swine manure biofuel created through hydrothermal liquefaction (HTL) as a promising fuel alternative. The process of HTL includes feeding biomass into a high pressure (8-20 MPa), high temperature (260-350^{o}C) reactor to create biocrude oil; however, this biocrude oil contains an unfeasible amount of gum content that inhibits its direct use as commercial fuel source for engines. In this sense, the goal of this study was to minimize the gum content of various viscous biocrude oil samples in order to meet the American Society for Testing and Materials (ASTM) fuel standards. A neutralization reaction of these HTL biocrude oil distillates, using a hydroxide solution (NaOH) to remove phenolic compounds residing in the samples, was conducted. The proposed hypothesis was that NaOH would react with phenols found in the biocrude oil samples resulting in a reduction of major compounds found in the gum content. In addition, an orthogonal study was conducted in order to investigate the effects of reaction temperatures (25^{o}C, 35^{o}C, 45^{o}C), reaction time (0.5 hr, 1 hr, 2 hr), concentrations of NaOH (1M, 2M, 5M) and swine manure distillate to NaOH weight ratios (2:1, 1:1, 1:3). Results included the discovery of ideal conditions for lowest gum content composition to be a reaction temperature of 45^{o}C, 2 hour reaction time, 2M of NaOH, and a 1:3 weight ratio of NaOH. Ultimately, with promising results the biocrude oil samples prove to be a potential alternative for petroleum diesel.

Bio-Medical Engineering III

Wednesday, March 14, 2018 (HH 005, WedC2)
Chair: Parinaz Fathi (University of Illinois at Urbana-Champaign)

3:30 PM Defined Host Guest Chemistry on Nanocarbon for Sustained Inhibition of Cancer (WedC2a) Fatemeh Ostadhossein, Santosh K. Misra (University of Illinois Urbana Champaign)

Signal transducer and activator of transcription factor 3 (STAT-3) is known to be overexpressed in cancer stem cells. Poor solubility and variable drug absorption are linked to low bioavailability and decreased efficacy. Many of the drugs regulating STAT-3 expression lack aqueous solubility; hence hindering efficient bioavailability. A theranostics nanoplatform based on luminescent carbon particles decorated with cucurbit[6]uril is introduced for enhancing the solubility of niclosamide, a STAT-3 inhibitor. The hostguest chemistry between cucurbit[6]uril and niclosamide makes the delivery of the hydrophobic drug feasible while carbon nanoparticles enhance cellular internalization. Extensive physicochemical characterizations confirm successful synthesis. Subsequently, the hostguest chemistry of niclosamide and cucurbit[6]uril is studied experimentally and computationally. In vitro assessments in human breast cancer cells indicate approximately twofold enhancement in IC50 of drug. Fourier transform infrared and fluorescence imaging demonstrate efficient cellular internalization. Furthermore, the catalytic biodegradation of the nanoplatforms occur upon exposure to human myeloperoxidase in short time. In vivo studies on athymic mice with MCF-7 xenograft indicate the size of tumor in the treatment group is half of the controls after 40 d. Immunohistochemistry corroborates the downregulation of STAT-3 phosphorylation. Overall, the host guest chemistry on nanocarbon acts as a novel arsenal for STAT-3 inhibition.

3:55 PM Lost in Translation: Mapping the Ribosomal Active Site in Vitro (WedC2b) Tasfia Azim, Anne d'Aquino, Adam J. Hockenberry, Michael C. Jewett (Northwestern University), Nikolay Aleksashin, Alexander Mankin (University of Illinois at Chicago)

The ribosome, a 2.5-MDa molecular machine that polymerizes amino acids into proteins, is the catalytic workhorse of the translation apparatus. The catalytic capacity of the translation machinery has attracted extensive efforts to repurpose it for novel functions. One key idea is that the natural translation machinery can be harnessed to synthesize polymers containing non-natural building blocks. Expanding the repertoire of ribosomal substrates and functions is a difficult task, however, because the requirement of cell viability severely constrains the alterations that can be made to the ribosome, a catalyst that sustains the life of a cell. In practice, these constraints have made the natural ribosome nearly unevolvable and, so far, no generalizable approach for modifying the catalytic peptidyl transferase center (PTC) of the ribosome has been advanced. We propose to address this grand challenge by using cell-free systems that harness the biosynthetic potential of cellular machines without using intact cells, thus removing cell viability constraints. Here, we use our in vitro ribosome synthesis, assembly, and translation system (termed iSAT) to generate variant ribosomes with mutations in the active site, and inquire how these modifications impact protein synthesis. The active site of the ribosome is composed solely of ribosomal RNA (rRNA). This rRNA is assembled into three key loops, which facilitate translation: the peptidyl transferase loop, the A-loop, and the P-loop. The peptidyl transferase loop plays a key role in positioning substrates, is involved with peptide stalling, and is a key target for antibiotic binding. The A- and P-loops flank the peptidyl transferase loop within the ribosomes active site. The A-loop is responsible for aminoacyl-tRNA interactions with the ribosome, and the P-loop is known to play a role in further facilitating peptide bond formation between amino acids. Because mutations to many of the nucleotides in these three active site loops confer lethal phenotypes, few to no studies exist in probing and fully characterizing them. Understanding the effects of single-base mutations on these active site nucleotides will provide insight into the basic biochemistry of these bases in translation, but also provide the groundwork for engineering the catalytic center of the ribosome. Using iSAT, we have assembled 180 different variant ribosomes possessing single-base substitutions of 23S rRNA nucleotides in these active site loops. By successfully quantifying full-length protein synthesis kinetics of iSAT-assembled wild type and mutant ribosomes, we unexpectedly found many key PTC mutations, which were expected to abolish ribosomal activity, still permitted full-length protein synthesis. We also assessed stop codon readthrough and ribosome assembly of these variants, as well as mapped mutant activity onto the ribosomes crystal structure. Our work provides the first and only comprehensive mapping of the impacts of every mutation within the ribosomes active site on protein synthesis. The understanding gained from these studies facilitates efforts to engineer and evolve ribosomes for synthetic biology.

4:20 PM Unsaturated Fatty Acid Ethyl Esters Inhibit Persister Cell Formation of Escherichia Coli and Pseudomonas Aeruginosa (WedC2c) Mengya Wang, Seok Hoon Hong (Illinois Tech)

Persisters are bacterial subpopulation that are dormant and survive under the antibiotic treatment without genetic modification. They are considered as one of the main reasons of recalcitrance of chronic bacterial infection. Although several mechanisms of persister formation have been proposed, it is not clear how cells enter the dormant state in the presence of antibiotics and how we can control persister cell formation effectively. It is known that cis-2-decenoic acid decreases persister formation as well as reverts the dormant cells to a metabolically active state. We reason that unsaturated fatty acids similar to cis-2-decenoic acid may be effective to control persister cells. In this study, we investigated persister formation of Escherichia coli with seven medium-chain fatty acids under different antibiotic treatment. We found that ethyl trans-2-decenoate, ethyl trans-2-octenoate, and ethyl cis-4-decenoate decreased the level of persister cell formation up to 110-fold when cells were exposed to ciprofloxacin or ampicillin antibiotics, while these fatty acid ethyl esters did not affect cell growth and pH of the culture. Also, these compounds are effective to inhibit persisters of pathogenic E. coli EDL933 and P. aeruginosa PAO1 strains. The mechanisms of persister inhibition by the fatty acids were revealed by analyzing RNA sequencing gene expression profiles affected by ethyl trans-2-decenoate during persister cell formation. This study guides us to identify new chemicals that influence bacterial dormancy and opens the development of novel strategies for combating infectious diseases. Keywords: persister cells, fatty acid ethyl esters, ethyl trans-2-decenoate, ethyl trans-2-octenoate, ethyl cis-4-decenoate, RNA sequencing

Transport Phenomena II

Wednesday, March 14, 2018 (HH 003, WedC3)
Chair: Caroline Szczepanski (Northwestern University)

3:30 PM Plowing-induced Segregation of Bidisperse Granular Mixtures (WedC3a) Vidushi Dwivedi, Alexander M. Fry, Paul B. Umbanhowar, Julio M. Ottino, Richard M. Lueptow (Northwestern University)

The lack of a thorough understanding of granular segregation makes it difficult to rationally address issues of design and scale-up, as well as control, in many industrial mixing processes. In this study, we perform a series of DEM simulations of a plowed bidisperse granular mixture to better understand segregation in the presence of temporally-periodic and spatially-localized driving. Our simulated system consists of a bed of particles with periodic boundaries in the streamwise and spanwise directions and a free surface, which makes the system effectively two-dimensional. A vertical wall (plow) located at the bottom of the particle bed and extending across the spanwise direction is displaced at constant velocity in the streamwise direction. Segregation is measured after each pass of the plow and characterized as a function of plow height and bed depth. Lower ratios of bed height to plow height result in higher initial rates of segregation and reach equilibrium faster than cases with higher ratios of bed height to plow height. A continuum-based segregation-advection-diffusion approach informed by the averaged kinematics measured in the DEM simulation may be useful to model the plowing-induced segregation.

3:55 PM Composite Membranes for Hemodialysis (WedC3b) Limin Lu, John Yeow (University of Waterloo)

Hemodialysis, developed in 1960s, has served as a treatment for patients with end stage renal disease. However, the 5 year mortality rate of hemodialysis patients is 65%. Research shows that some protein-bound toxins, which cannot be cleared by hemodialysis, play an important role in mortality of dialysis patients. In order to improve the mortality rate of dialysis patients, we created polyethersulfone-zeolites composite dialysis membranes, which can remove both water-soluble toxins and protein bond toxins. Experiments showed that these membranes can adsorb 4948 μg creatinine per g membranes. The effects of pH and salt on zeolites adsorption and desorption of creatinine were also studied in order to infer the membranes adsorption mechanism. We found that acidic environments enhance zeolites creatinine adsorption while alkaline environments weaken it. The existence of various cations also decreases zeolites creatinine adsorption. Indoxyl sulfate, an important toxin in causing reno-cardiovascular syndromes, was chosen as a representative of protein-bound toxins. Experiments show that zeolite-PES membranes can adsorb 550 μg indoxyl sulfate per g membranes, and indicate that the adsorption mechanism is likely to be electrostatic attraction.

4:20 PM Control of Polymorphism in Continuous Crystallization (WedC3c) Shivani Kshirsagar, Zoltan Nagy (Purdue University)

Control of polymorphism in ortho-aminobenzoic acid (OABA) to form 1 and form 2 in continuous crystallization is studied. The effect of operating parameters on the polymorphic form is studied and will be presented in the talk. Some batch crystallization experiments were conducted to decide ranges of operating parameters in the continuous crystallization.

Wednesday Dinner Keynote

Wednesday, March 14, 2018 (Ballroom)
Chair: Satish Parulekar (Illinois Tech)

7:00 PM Metabolic Complexity. Is there Music Behind it? Doraiswami Ramkrishna (Purdue University)

The complexity of metabolic networks would appear to fit in more appropriately with a cacophonic scenario than anything remotely musical. However, this talk will attempt to show that a mathematical view can be had of this complex process in which the phenomenon of metabolic regulation can be likened to the conductor of a symphonic orchestra summoning combinations of instruments representing metabolic reactions towards superlative music. It will be the objective of this seminar to let this analogy lead the discussion of a cybernetic theory of cellular metabolism which interprets the diversity of gene expression as a targeted effort to maximize the organisms survival.

AIChE Midwest Regional Conference
High School Outreach Program

This special high school program is being run in parallel with the American Institute of Chemical Engineers (AIChE) 10th 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!

8:45-9:30	**Engineering Expo** (Gallery Lounge) - Meet with current engineering students and see some of their projects
9:30-11:00	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 Bob Anderson (Illinois Tech) **Team Building Exercise** (Expo Room) - Work with other students to complete a hands-on engineering-related task
11:00-11:30	**Engineering Panel Session** (Auditorium) - Learn about the day-to-day activities of practicing engineers and engineering students. Time to ask your most burning questions.
11:30-12:15	**Engineering Lunch** (Ballroom and Expo Room) - Opportunity for one-on-one discussions with engineering professionals and students.
12:15-1:00	**Keynote Speaker** (Auditorium) - Valarie King-Bailey, M.B.A – Chief Executive Officer, OnShore Technology Group
1:00-2:00	**Tours of the Illinois Tech Campus** (Meet at Gallery Lounge)

Valarie King-Bailey, M.B.A.
Valarie King-Bailey is the CEO of OnShore Technology Group, an independent Chicago-based consultancy specializing in Independent Validation and Verification (IV&V) products and solutions. OnShore's product, ValidationMaster™ is the first fully integrated Enterprise Validation Management system on the market. ValidationMaster™ was recognized by CIO Review Magazine as one of the top 20 most promising technologies for life sciences in 2015. OnShore led the development of the first FDA Validation Toolkit for Microsoft Dynamics AX and Microsoft NAV. Valarie has worked for leading global companies such as QUMAS Limited (Ireland), EMC/Documentum, Abbott Laboratories, and U.S. Steel – South Works. At QUMAS, an Irish-based software company, she served as Chief Marketing Officer where she was responsible for all global tactical and strategic marketing initiatives in addition to the development of their validation toolkit. Valarie founded OnShore Technology Group in 2004. OnShore Technology Group recently won the American Express/Count Me In M3 Award and the Madam C.J. Walker Outstanding Business Award (2008). She also received a nomination for Ernst & Young Entrepreneur of the Year award in 2006. Ms. King- Bailey holds an M.B.A. in Information Systems from Keller Graduate School of Management (1985) and a B.S. in Civil and Environmental Engineering from the University of Wisconsin – Madison (1982). She is a member of the American Society of Civil Engineers, Society of Women Engineers, National Girls Collaborative Project for STEM education, Regulatory Affairs Professional Society (RAPS), and a U.W. College of Civil Engineering Advisory Board Member.

HS Outreach Organizing Committee
Chair: Ellen Kloppenborg (UOP/Honeywell)
Co-Chair Programming: Akshar Patel (Illinois Tech)
Co-Chairs Programming/Volunteers: Paige Grons, Sarah O'Donnell (Illinois Tech)

AIChE Midwest Regional Conference

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