13th Annual
AIChE Midwest Regional Conference

March 17-18, 2021

https://www.aiche.org/conferences/midwest-regional-conference/2021

**Organized by the AIChE Chicago Local Section and
AIChE Global**

THANK YOU!

The following organizations generously contributed to the AIChE Chicago's student outreach programs in 2020.

AIChE Midwest Regional Conference

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 13th year. Organized by the **AIChE Chicago Local Section** and **AIChE Global**, 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:

5 Keynote Lectures:
- **William Schneider**, *Professor and Chair, Department of Chemical and Biomolecular Engineering, University of Notre Dame*
- **Cathy Tway,** *Technology & Applications Director, Catalyst Technologies, Johnson Matthey*
- **Sohail Murad,** *Professor and Chair, Department of Chemical and Biological Engineering, Illinois Institute of Technology*
- **Marius Stan,** *Senior Scientist and Leader of Intelligent Materials Design, Applied Materials Division, Argonne National Laboratory*
- **Ray Mentzer**, *Professor of Engineering Practice and Executive Director of Purdue Process Safety & Assurance Center, Davidson School of Chemical Engineering, Purdue University*

The virtual conference contains **12 technical sessions** featuring over **30 oral presentations** as well as a **career development session**. 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 **Elizabeth Corson** (Stanford University) as keynote speaker and includes a special virtual luncheon where students can interact with practicing chemical engineers. On behalf of the conference planning committee, we welcome you to the 13th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Robert Tsai	Matthew Walters	Hakim Iddir
Conference Chair	Conference Co-Chair	Program Chair
Honeywell UOP	Exponent	Argonne National Laboratory

AIChE Midwest Regional Conference
Program at a Glance

Wednesday, March 17, 2021

8:30 AM – 9:30 AM	**Morning Keynote** (WeK1) - William Schneider*, Professor and Chair, Department of Chemical and Biomolecular Engineering, University of Notre Dame*
9:30 AM – 9:45 AM	**Networking Break**
9:45 AM – 11:45 AM	**Technical Sessions** - *Catalysis and Reaction Engineering* (WeA1) - *Fluid Properties, Fluid Dynamics, and Transport Phenomena* (WeA2)
11:45 AM – 12:45 PM	**Networking/ Lunch Break**
12:45 PM – 1:45 PM	**Afternoon Keynote** (WeK2) - Cathy Tway*, Technology & Applications Director, Catalyst Technologies, Johnson Matthey*
1:45 PM – 2:00 PM	**Networking Break**
2:00 PM – 3:30 PM	**Technical Sessions** - *Climate Solutions* (WeB1) - *Energy Storage I* (WeB2)
3:30 PM – 3:45 PM	**Networking Break**
3:45 PM – 5:15 PM	**Technical Sessions** - *Biorefining Technology* (WeC1) - *Energy Storage II* (WeC2)
5:15 PM – 5:30 PM	**Networking Break**
5:30 PM – 7:30 PM	**AIChE Chicago March Dinner Meeting**
6:00 PM – 7:00 PM	**Dinner Keynote** (WeK3) - Sohail Murad*, Professor and Chair, Department of Chemical and Biological Engineering, Illinois Institute of Technology*

AIChE Midwest Regional Conference

Program at a Glance

Thursday, March 18, 2021

8:30 AM – 9:30 AM	**Morning Keynote** (ThK1) - Marius Stan*, Senior Scientist and Leader of Intelligent Materials Design, Applied Materials Division, Argonne National Laboratory*
9:30 AM – 9:45 AM	**Networking Break**
9:45 AM – 11:15 AM	**Technical Sessions** - *Machine Learning and Optimization* (ThA1) - *Process Safety and Occupational Health I* (ThA2)
11:15 AM – 12:45 PM	**Networking / Lunch Break**
11:30 AM – 12:30 PM	**Lunch with High School Outreach Participants** [optional signup]
12:45 PM – 1:45 PM	**Afternoon Keynote** (ThK2) - Ray Mentzer*, Professor of Engineering Practice and Executive Director of Purdue Process Safety & Assurance Center, Davidson School of Chemical Engineering, Purdue University*
1:45 PM – 2:00 PM	**Networking Break**
2:00 PM – 3:30 PM	**Technical Sessions** - *Advances in Refining* (ThB1) - *Process Safety and Occupational Health II* (ThB2)
3:30 PM – 3:45 PM	**Networking Break**
3:45 PM – 5:15 PM	**Technical Sessions** - *Environmental Compliance and Remediation* (ThC1) - *Biomedical, Pharmaceutical, and Nano-Engineering* (ThC2) - *YP Session: Job Search Skills* (ThC3)
5:15 PM – 6:30 PM	**Poster Session** (ThP1)
6:30 PM – 8:30 PM	**Young Professional Virtual Networking Social**

AIChE Midwest Regional Conference

Keynote Speakers

Wednesday Morning Keynote: 8:30 AM Wednesday, March 17, 2021

William Schneider*, Professor and Chair, Department of Chemical and Biomolecular Engineering, University of Notre Dame*

Presentation Title: ***Models and Opportunities in Plasma Catalysis***

Biographical Sketch: *Bill Schneider's expertise is in chemical applications of density functional theory (DFT) simulations. After receiving his Ph.D. in Inorganic Chemistry from the Ohio State University, he began his professional career in the Ford Motor Company Research Laboratory working on a variety of probl ems related to the environmental impacts of automobile emissions. At Ford he developed an interest in the catalytic chemistry of NOx for diesel emissions control, and he has published extensively on the chemistry and mechanisms of NOx decomposition, selective catalytic reduction, trapping, and oxidation catalysis. In 2004 he joined the Chemical and Biomolecular Engineering faculty at the University of Notre Dame as an Associate Professor. At Notre Dame he has continued his research into the theory and molecular simulation of heterogeneous catalysis, with particular emphasis on reaction environment effects on catalytic materials and their implications for mechanism and reactivity. He was named the H. Clifford and Evelyn A. Brosey Chair in 2016 and Dorini Family Chair and Chair of the Department of Chemical and Biomolecular Engineering in 2020. He has co-authored 200 articles and book chapters, is a Fellow of the American Association for the Advancement of Science, is an Executive Editor of The Journal of Physical Chemistry, and was the 2018 recipient of the Giuseppe Parravano Award of the Michigan Catalysis Society.*

Wednesday Afternoon Keynote: 12:45 PM Wednesday, March 17, 2021

Cathy Tway, *Technology & Applications Director, Catalyst Technologies, Johnson Matthey*

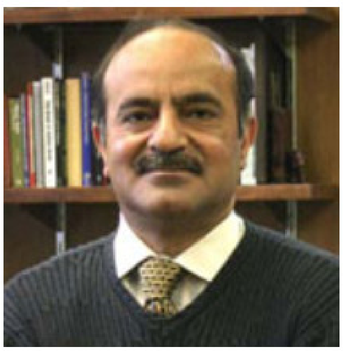
Presentation Title: ***The Future Ain't What It Used To Be***

Biographical Sketch: *Cathy Tway is the Technology and Applications Director for Catalyst Technologies in Johnson Matthey. In her role, Cathy is responsible for a global team of scientists and engineers specializing in catalysis, process technologies, and engineering design. She ensures customer driven R&D and engineering is delivered efficiently and provides technical input, oversight, and direction.*

Johnson Matthey (JM) is an international specialty chemicals company and a leader in sustainable technologies. Established in 1817, the company has a long history of innovation in advanced materials and technologies. JM's vision is for a world that is cleaner and healthier; today and for future generations. The company uses its expertise in advanced materials and technology to innovate and improve solutions that are valued by customers, optimize the use of natural resources and enhance the quality of life for millions of people around the world. Within JM, the Catalyst Technologies Business Unit supplies catalysts, absorbents and licensed processes to enable its customers to achieve chemical transformations with greater efficiency and reduced environmental impact.

Prior to joining Johnson Matthey, Cathy held positions at Dow, Celanese, Solutia, and Akzo Nobel, holding both R&D leadership and individual contributor roles. Her more than 25 years of industrial experience covers the entire catalyst project life cycle including front-end opportunity identification and creation of new technologies, process scale-up, commercialization and plant support. Over her career, Cathy has commercialized two new inorganic materials and four catalyst technologies, with two of these processes still in use today. She has served on numerous review panels, boards and committees including the committee for the National Academies of Sciences, Engineering, and Medicine consensus study report on "Gaseous Carbon Waste Streams Utilization." Cathy earned her BS degree in chemistry from Wichita State University and her Ph.D. in physical inorganic chemistry from the University of Nebraska-Lincoln.

Wednesday Dinner Keynote: 6:00 PM Wednesday, March 17, 2021



Sohail Murad*, Professor and Chair, Department of Chemical and Biological Engineering, Illinois Institute of Technology*

Presentation Title: ***Using Molecular Modeling for Screening and Optimizing Membrane Based Separation Processes***

Biographical Sketch: *Dr. Sohail Murad is Professor and Department Chair of Chemical and Biological Engineering at the Illinois Institute of Technology. Prior to this he was Head of Chemical Engineering at University of Illinois at Chicago, where he joined the faculty in 1979 after receiving a PhD from Cornell University, Ithaca, NY. He spent 1981-82 at Exxon Research and Engineering Company at Florham Park, New Jersey, while on a leave of absence from the university. He was an ARO Research Fellow at the Ballistics Research Laboratory in 1985. He is the author of over 150 archival research publications and book chapters. He is/has been a member of the Editorial Advisory Board of* Computer Applications in Engineering Education, Scientific Journals International and Research Letters in Chemical Engineering*. His research is focused on alternate energy and its efficient utilization, computational molecular modeling of fluids on membrane surfaces and pores and on heat and mass flows in nanosystems. It has been funded by the US National Science Foundation, US Department of Energy, US Army Research Office, American Chemical Society, IBM, Dow Chemical Company, Sun Microsystems, Microsoft, and other private and public funding agencies. He is an elected fellow of the American Institute of Chemical Engineers, and member of several other professional societies. He holds honorary faculty positions at Nanjing University (China), Petra University (Jordan), and University of Karachi (Pakistan). He has given many keynote talks at national and international symposia, and has served on panels of the National Science Foundation, Department of Energy, Department of Defense, Environmental Protection Agency, etc.*

Thursday Morning Keynote: 8:30 AM Thursday, March 18, 2021

Marius Stan*, Senior Scientist and Leader of Intelligent Materials Design, Applied Materials Division, Argonne National Laboratory*

Presentation Title: ***Science and Society***

Biographical Sketch: *Dr. Marius Stan is a Senior Scientist and Leader of Intelligent Materials Design in the Applied Materials Division at Argonne National Laboratory. He is also a Senior Fellow at University of Chicago and Northwestern University. Marius and his team use artificial intelligence (AI) and high-performance, multi-scale computer simulations to understand and predict physical and chemical properties of multi-component metals and ceramics. The applications include energy production (nuclear fuels and reactor materials), energy storage (batteries) and electronics. The team also uses AI to optimize complex processes for manufacturing applications such as 3-D printing and flame spray pyrolysis. Marius has extensively published in the scientific literature, holds several patents, and is currently writing a book on modeling and simulation. He is also an author of short-stories and poetry. Some will recognize him as an actor, portraying* Bogdan *in the award-winning TV series* Breaking Bad*.*

Thursday Afternoon Keynote: 12:45 PM Thursday, March 18, 2021

Ray A. Mentzer, *Professor of Engineering Practice and Executive Director of Purdue Process Safety & Assurance Center, Davidson School of Chemical Engineering, Purdue University*

Presentation Title: ***Process Safety Update - Training, Research, ... Where Are We Headed?***

Biographical Sketch: *Ray is a Professor of Engineering Practice in the Charles Davidson School of Chemical Engineering at Purdue since 2016, where he teaches the required senior level 'Chemical Process Safety' course and is Executive Director of the Purdue Process Safety & Assurance Center. The Center oversees a wide variety of process safety research at PhD, MS and UG levels, with a dozen faculty and about three dozen students engaged. Previously, he taught at Texas A&M and was part of the Mary Kay O'Connor Process Safety Center for seven years. Earlier he had a 28-year career with ExxonMobil, with over a dozen assignments, with experience in research, facility design, operations, finance, public affairs, and safety & environment. He has a BS from the University of Illinois, and MS & PhD from Purdue - all in Chemical Engineering.*

AIChE Midwest Regional Conference

Session Presentations

Wednesday, March 17, 2021

Wednesday Morning Keynote Session
Wednesday, March 17, 2021 (**WeK1**)
8:30 AM **LS Chair's Welcome**
Jeffrey Zalc (BP)
8:35 AM **Keynote Introduction**
Hakim Iddir (Argonne National Laboratory)
8:40 AM **Models and Opportunities in Plasma Catalysis**
William Schneider (University of Notre Dame)

Catalysis and Reaction Engineering
Wednesday, March 17, 2021 (**WeA1**)
Chair: *Aditya Prajapati* (University of Illinois at Chicago)
Co-chair: *Iman Nezam* (Georgia Institute of Technology)
9:45 AM **Synthesis, Characterization and Analysis of TiO2/ZnO Composites Photocatalytic Thin Films for Diurnal Fuel Vapor Degradation in Automobile** (WeA1a)
Ibrahim Sanusi (Miami University)
10:10 AM **Improving the Selectivity of Epoxide Ring-Opening Using Diol Co-Catalysts for Polyurethane Applications** (WeA1b)
Mihir Bhagat (Northwestern University), *Matthew Belowich* (The Dow Chemical Company), *Charmaine Bennett* (Northwestern University), *Linda Broadbelt* (Northwestern University), *Gao-Fong Chang* (Northwestern University), *SonBinh Nguyen* (Northwestern University), *Justin Notestein* (University of California, Berkeley), *Arjun Raghuraman* (The Dow Chemical Company)
10:35 AM **Controlled Oxygen-Peroxide Chemistry in LI-Oxygen Batteries By Molecular Redox Mediators** (WeA1c)
Erik Askins (University of Illinois at Chicago), *Ksenija Glusac* (University of Illinois at Chicago), *Marija Zoric* (University of Illinois at Chicago)
11:00 AM **Grafting Synthesis of Silica-Supported Boron** (WeA1d)
Melissa Cendejas (University of Wisconsin-Madison), *Rick W. Dorn* (Iowa State University), *Ive Hermans* (University of Wisconsin-Madison), *William P. McDermott* (University of Wisconsin-Madison), *Aaron Rossini* (Iowa State University)
11:25 AM **Live Session Q&A** (WeA1e)

Fluid Properties, Fluid Dynamics, and Transport Phenomena
Wednesday, March 17, 2021 (**WeA2**)
Chair: *Joel Paustian* (Honeywell UOP)
Co-Chair: *Shri Dawande* (Illinois Institute of Technology)
9:45 AM **CFD Modeling of a Bioreactor** (WeA2a)
Reza Mostofi (Honeywell UOP), *Azita Ahmadzadeh* (Honeywell UOP), *Steve Poklop* (Honeywell UOP)
10:10 AM **Design of a Fully Integrated Artificial Photosynthetic System for a Moisture-Gradient CO2 Capture and Reduction** (WeA2b)
Aditya Prajapati (University of Illinois at Chicago), *Meenesh R. Singh* (University of Illinois at Chicago)
10:35 AM **Maxwell Viscoelasticity of Complex Fluids Mixtures** (WeA2c)
Guler Bengusu Tezel (Bolu Abant Izzet Baysal University)
11:00 AM **Modeling and Numerical Simulation of Concentrated Solar Energy Storage in a Packed Bed of Silicon Carbide Particles** (WeA2d)
Zeyuan Gao (Illinois Institute of Technology), *Javad Abbasian* (Illinois Institute of Technology), *Hamid Arastoopour* (Illinois Institute of Technology) [**canceled**]
11:25 AM **Live Session Q&A** (WeA2e)

Wednesday Afternoon Keynote Session
Wednesday, March 17, 2021 (**WeK2**)
12:45 PM **Keynote Introduction**
Robert Tsai (Honeywell UOP)
12:50 PM **The Future Ain't What It Used To Be**
Cathy Tway (Johnson Matthey)

Climate Solutions
Wednesday, March 17, 2021 (**WeB1**)
Chair: *Dennis O'Brien* (Jacobs Engineering)
2:00 PM **Power, Natural Gas, and the Impacts of Carbon Pricing** (WeB1a)

Thomas Rausch (CWE)

2:25 PM **Dispassionate Deliberate Collaboration Can Resolve Global Warming and Its Climate Change Effects** (WeB1b)
Thomas Rehm (STS Chair)

2:50 PM **Clues to Climate Mitigation Priorities from Global Greenhouse Gas Budgets** (WeB1c)
Gavin McNicol (University of Illinois at Chicago), *Max Berkelhammer* (University of Illinois at Chicago)

3:15 PM **Live Session Q&A** (WeB1d)

Energy Storage I

Wednesday, March 17, 2021 (**WeB2**)
Chair: *Hakim Iddir* (Argonne National Laboratory)
Co-Chair: *Juan Garcia* (Argonne National Laboratory)

2:00 PM **Strain-Driven Surface Reconstruction and Cation Segregation in Layered Li(Ni1-x-yMnxCoy)O2 (NMC) Cathode Materials** (WeB2a)
Juan Garcia (Argonne National Laboratory)

2:25 PM **Structure-Activity Relationships in Lithium Ion Batteries: Solid State NMR Characterization of Lithium-Ion Cathodes and Anodes** (WeB2b)
Fulya Dogan (Argonne National Laboratory)

2:50 PM **Understanding the (de)Lithiation Mechanism of Pb-Based Nanocomposite Anode for High Performance Lithium-Ion Batteries** (WeB2c)
Jinhyup Han (Argonne National Laboratory), *Seong-Min Bak* (Brookhaven National Laboratory), *Jihyeon Gim* (Argonne National Laboratory), *Xiaobing Hu* (Northwestern University), *Christopher Johnson* (Argonne National Laboratory), *Youngsik Kim* (Ulsan National Institute of Science and Technology), *Eungje Lee* (Argonne National Laboratory), *Jehee Park* (Argonne National Laboratory), *Seoung-Bum Son* (Argonne National Laboratory), *Chi Cheung Su* (Argonne National Laboratory), *Cesar Villa* (Northwestern University)

3:15 PM **Live Session Q&A** (WeB2d)

Biorefining Technology

Wednesday, March 17, 2021 (**WeC1**)
Chair: *Belma Demirel* (BP)

3:45 PM **The Pursuit of a Cleaner Healthier World through Bio Renewables** (WeC1a)
Grace Rhoades (Johnson Matthey)

4:10 PM **Techno-Economic Analysis of the Modified Mixalco Process** (WeC1b)
Chloe Simchick (Milwaukee School of Engineering) [**canceled**]

4:35 PM **OPEN** (WeC1c)

5:00 PM **Live Session Q&A** (WeC1d)

Energy Storage II

Wednesday, March 17, 2021 (**WeC2**)
Chair: *Juan Garcia* (Argonne National Laboratory)
Co-chair: *Hakim Iddir* (Argonne National Laboratory)

3:45 PM **A Lithium Accounting Model with Unstable Electrolytes: Protocol Dependence, Invisible Processes, and the Consequences of Reactivity** (WeC2a)
Adam Tornheim (Argonne National Laboratory), *Daniel O'Hanlon* (Argonne National Laboratory)

4:10 PM **NiMn5050-Based Cathodes As Next Generation Cathodes for Lithium-Ion Battery** (WeC2b)
Anh Vu (Argonne National Laboratory), *Jason Croy* (University of Central Florida), *Yang Ren* (Argonne National Laboratory)

4:35 PM **Lead-Based Nanocomposites As Anode Material for Sodium-Ion Batteries** (WeC2c)
Jehee Park (Argonne National Laboratory), *Shabbir Ahmed* (Argonne National Laboratory), *Seong-Min Bak* (Brookhaven National Laboratory), *Jihyeon Gim* (Argonne National Laboratory), *Jinhyup Han* (Argonne National Laboratory), *Christopher Johnson* (Argonne National Laboratory), *Youngsik Kim* (Ulsan National Institute of Science and Technology), *Eungje Lee* (Argonne National Laboratory)

5:00 PM **Live Session Q&A** (WeC2d)

Local Section Dinner and Dinner Keynote

Wednesday, March 17, 2021 (**WeK3**)

5:30 PM **Networking**

5:45 PM **Local Section Announcements**
Jeffrey Zalc (BP)

5:55 PM **Keynote Introduction**
Chris Nicholas (Honeywell UOP)

6:00 PM **Using Molecular Modeling for Screening and Optimizing Membrane Based Separation Processes**
Sohail Murad (Illinois Institute of Technology)

AIChE Midwest Regional Conference
Session Presentations
Thursday, March 18, 2021

__Thursday Morning Keynote Session__
Thursday, March 18, 2021 (**ThK1**)
8:30 AM **Recognition for Volunteers from the Conference Chair**
Robert Tsai (Honeywell UOP)
8:35 AM **Keynote Introduction**
Hakim Iddir (Argonne National Laboratory)
8:40 AM **Science and Society**
Marius Stan (Argonne National Laboratory)

__Machine Learning and Optimization__
Thursday, March 18, 2021 (**ThA1**)
Chair: *Joshua Gabriel* (Argonne National Laboratory)
Co-Chair: *Aditya Prajapati* (University of Illinois at Chicago)
9:45 AM **Machine Learning Force Fields for Li-Ion Cathodes** (ThA1a)
Joshua Gabriel (Argonne National Laboratory), *Juan Garcia* (Argonne National Laboratory), *Hakim Iddir* (Argonne National Laboratory), *John Low* (Argonne National Laboratory), *Noah Paulson* (Argonne National Laboratory), *Marius Stan* (Argonne National Laboratory)
10:10 AM **Cost Productivity Approach to Industry 4.0 Cybersecurity** (ThA1b)
Pranav Patel (ResiliAnt by MediTechSafe), *Prerak Patel* (ResiliAnt)
10:35 AM **Artificial Intelligence (AI) – Machine Learning (ML) Based Framework for Optimal Design of Interfacially Polymerized Thin Film Nanocomposite Membranes for Desalination** (ThA1c)
Jasneet Kaur Pala (BITS Pilani K K Birla Goa Campus) [**canceled**]
11:00 AM **Live Session Q&A** (ThA1d)

__Process Safety and Occupational Health I__
Thursday, March 18, 2021 (**ThA2**)
Chair: *David Hietala* (Exponent)
Co-Chair: *Jessica Morris* (Exponent)
9:45 AM **Why Storage Tanks Leak and How to Stay Safe** (ThA2a)
Jessica Morris (Exponent), *Ryan Hart* (Exponent), *Delmar Morrison* (Exponent)
10:10 AM **Mechanical Integrity for Aging Process Facilities - Ensuring Safe Operations over Time** (ThA2b)
Robert Weber (PSRG Inc.)
10:35 AM **Combustible Dust Hazards and Spray Drying Systems – Understanding NFPA 61's New Requirements in a Dust Hazard Analysis** (ThA2c)
Sean Dee (Exponent), *Brenton Cox* (Exponent), *Russell Ogle* (Exponent), *Matthew Walters* (Exponent)
11:00 AM **Live Session Q&A** (ThA2d)

__Thursday Afternoon Keynote Session__
Thursday, March 18, 2021 (**ThK2**)
12:45 PM **Keynote Introduction**
Matthew Walters (Exponent)
12:50 PM **Process Safety Update - Training, Research, ... Where Are We Headed?**
Ray Mentzer (Purdue University)

__Advances in Refining__
Thursday, March 18, 2021 (**ThB1**)
Chair: *Belma Demirel* (BP)
Co-chair: *Shahineze Saada* (Honeywell UOP)
2:00 PM **Reducing Octane Loss – Solutions for FCC Gasoline Post-Treatment Services** (ThB1a)
Claus Brostrom Nielsen (Haldor Topsoe A/S)
2:25 PM **Premium Performance Delivered in Challenging Middle Distillates Hydrotreating Operations** (ThB1b)
Aaron Joss (Albemarle)
2:50 PM **Ultra-High Temperature Resistant Preformed Particle Gels for Enhanced Oil Recovery** (ThB1c)
Buddhabhushan Salunkhe (Missouri University of Science and Technology), *Baojun Bai* (Missouri University of Science and Technology), *Thomas Schuman* (Missouri University of Science and Technology)
3:15 PM **Live Session Q&A** (ThB1d)

__Process Safety and Occupational Health II__
Thursday, March 18, 2021 (**ThB2**)
Chair: *Jessica Morris* (Exponent)
Co-chair: *David Hietala* (Exponent)

2:00 PM **Understanding Fire Hazards in Inert Cryogenic Systems** (ThB2a)
Ehson Fawad Nasir (Exponent), *Sean Dee* (Exponent), *Suzanne Smyth* (Exponent), *Nicholas A. Traina* (Exponent)

2:25 PM **Common Cause Failure – What Are They and How to Mitigate Them?** (ThB2b)
Tekin Kunt (PSRG Inc.)

2:50 PM **Means to Achieve Backflow Prevention of Hazardous Chemicals from Process Vessels to Utility Pipelines** (ThB2c)
Deepak Sharma (Bayer US)

3:15 PM **Live Session Q&A** (ThB2d)

Environmental Compliance and Remediation
Thursday, March 18, 2021 (**ThC1**)
Chair: *Jarad Champion* (Geosyntec)

3:45 PM **Destructive Technologies for per- and Polyfluoroalkyl Substances (PFAS)** (ThC1a)
Mary Ensch (Geosyntec)

4:10 PM **Improving Membrane Fouling Resistance in Water Filtration with Polyelectrolyte Complex Sacrificial Layers** (ThC1b)
Yechan Wong (Geosyntec)

4:35 PM **Are Catastrophes Affecting Compliance?** (ThC1c)
Katherine Culbert (K and K Process)

5:00 PM L**ive Session Q&A** (ThC1d)

Biomedical, Pharmaceutical, and Nano-Engineering
Thursday, March 18, 2021 (**ThC2**)
Chair: *Abhinav Bhushan* (Illinois Institute of Technology)
Co-chair: *Seok Hoon Hong* (Illinois Institute of Technology)

3:45 PM **Polymersome Encapsulation of a High Logp Protein-Protein Interaction Inhibitor to Achieve Increased Solubility and Therapeutic Index** (ThC2a)
Yu Tian (University of Delaware), *James L. LaBelle* (University of Chicago), *Mathew R. Schnorenberg* (University of Chicago), *Matthew V. Tirrell* (University of Chicago)

4:10 PM **Engineering *Shewanella Oneidensis* for Bisphenol a Degradation and Biofilm Formation** (ThC2b)
Jiacheng Zhou (Illinois Institute of Technology), *Seok Hoon Hong* (Illinois Institute of Technology)

4:35 PM **Mechanical and Structural Characterization of Thin Films** (ThC2c)
Mark Haase (Anton Paar) [**canceled**]

5:00 PM L**ive Session Q&A** (ThC2d)

YP Session: Job Search Skills
Thursday, March 18, 2021 (**ThC3**)
Chair: *Ruben Barajas* (Honeywell UOP)
Co-chair: *Connor Wegner* (Leister Technologies)

3:45 PM **Pre-Scheduled Meetings** (ThC3a)

Poster Session
Thursday, March 18, 2021 (**ThP1**)

5:15 PM **Poster Session**

Poster 1 **Digitalization of Process Safety - Utilizing Wearables to Conduct Remote Activities Safely** (ThP1a)
Robert Weber (PSRG, Inc.)

Poster 2 **Techno Economic Analysis of the Modified Mixalco Process** (ThP1b)
Brooke Zidek (Milwaukee School of Engineering), *Chloe Simchick* (Milwaukee School of Engineering)

Poster 3 **Predicting Reaction Mechanism of Electrochemical CO2 Reduction Using Machine Learning** (ThP1c)
Aditya Prajapati (University of Illinois at Chicago)

Poster 4 **Cost Productive Cybersecurity Approach to Securing Plant Operations** (ThP1d)
Pranav Patel (ResiliAnt)

Presentation Abstracts

Wednesday, March 17, 2021

Wednesday Morning Keynote Session
Wednesday, March 17, 2021 (**WeK1**)

8:40 AM Models and Opportunities in Plasma Catalysis

William Schneider (University of Notre Dame)

Heterogeneous catalysis is essential to industrial chemical processes, from those that transform petroleum into fuels and chemicals to those, like the Haber Bosch process, that create fertilizers to feed the planet. The first heterogeneous catalysts were discovered empirically and improved through Edisonian experimentation. Within the last twenty years or so, however, the field has been transformed through the advent of catalysis science, which, using high fidelity synthesis and characterization coupled with molecular-level models, is able to understand and predict catalytic function. Catalysis science has revealed that the most common heterogeneous catalysts present a tableau of reactivity limited by intrinsic correlations between the various reaction steps that make up a surface catalytic reaction. Coupling of heterogeneous catalysts with non-thermal plasmas offers the potential to break these constraints. While empirical evidence suggests that such combinations can enhance apparent catalytic function relative to plasmas or catalysts alone, the absence of basic models to rationalize this behavior and guide material and plasma selection has limited progress. In this talk I will describe recent work to bridge this gap through the development of models that highlight the potential origins and consequences of combining non-thermal plasmas and catalysts, all in the context of nitrogen fixation.

Catalysis and Reaction Engineering
Wednesday, March 17, 2021 (**WeA1**)
Chair: *Aditya Prajapati* (University of Illinois at Chicago)
Co-chair: *Iman Nezam* (Georgia Institute of Technology)

9:45 AM Synthesis, Characterization and Analysis of TiO2/ZnO Composites Photocatalytic Thin Films for Diurnal Fuel Vapor Degradation in Automobile (WeA1a)

Ibrahim Sanusi (Miami University)

The specific purpose of this project is to investigate ZnO/TiO2 composites as photocatalytic films for fuel vapor oxidation. Pure TiO2, pure ZnO and combinations of them to make composite photocatalysts will be synthesized, characterized and dip coated as thin films in a photocatalytic reactor. The photocatalytic oxidation of VOCs in air will be used to assess the relative photocatalytic activity of the ZnO/TiO2 composite films. A statistical factorial design will be conducted to analyze the effect of reactor well depth, catalyst composition, and ethanol flowrate per unit area on the photocatalytic oxidation (degradation) of ethanol. As motivated by the US EPA P3 (People, Prosperity, and Planet), to design environmental solutions for a sustainable future, the overall aim of this project is to design a novel micro-meso-structure UV Led photocatalytic reactor to be incorporated into modern automobiles for the degradation of volatile organic compounds (VOCs) resulting from diurnal fuel vapor emissions.

10:10 AM Improving the Selectivity of Epoxide Ring Opening Using Diol Co-Catalysts for Polyurethane Applications (WeA1b)

Mihir Bhagat (Northwestern University), *Matthew Belowich* (The Dow Chemical Company), *Charmaine Bennett* (Northwestern University), *Linda Broadbelt* (Northwestern University), *Gao-Fong Chang* (Northwestern University), *SonBinh Nguyen* (Northwestern University), *Justin Notestein* (University of California, Berkeley), *Arjun Raghuraman* (The Dow Chemical Company)

Epoxide ring-opening is key for the synthesis of many intermediates and compounds. Industrially, it is employed with alcohol initiators for manufacturing polyether polyols, which are primary feedstocks for polyurethane polymers. This reaction occurs in the presence of a catalyst and generally yields primary

(P1) and secondary alcohol (P2) products, with the latter being undesired due to their low reactivity. However, most conventional industrial catalysts such as KOH and DMC catalysts are poorly selective and yield P1:P2 ratios <0.1, which necessitates additional processing to achieve the desired P1 content. In contrast, we saw that tris(pentafluorophenyl)borane [B(C6F5)3], or BCF, is a highly Lewis acidic catalyst that offers fast rates and P1:P2 selectivities as high as 3.5:1[1]. Moreover, BCF also forms active adducts with residual water, thereby creating H2O-mediated catalysis cycles. We initially proposed that, while one of the protons on the BCF-OH2 adduct can participate in ring-opening, the other proton could be leveraged to modify selectivity at the former, via the addition of a suitable hydrogen bond acceptor (HBA). In this work, we confirm this concept using experiments and theory and explain the role of reaction products P1 and P2 on the selectivity of BCF-catalyzed epoxide ring-opening [2]. Additionally, we were also able to bring about significant enhancements to regioselectivity by adding 1,2-diol HBAs as co-catalysts [3]. We further expand this effect to include a range of diols, substrates and nucleophiles. Having established the basis for this phenomenon, these findings will further guide the discovery of other HBA classes for this reaction.

10:35 AM Controlled Oxygen-Peroxide Chemistry in LI-Oxygen Batteries By Molecular Redox Mediators (WeA1c)

Erik Askins (University of Illinois at Chicago), *Ksenija Glusac* (University of Illinois at Chicago), *Marija Zoric* (University of Illinois at Chicago)

Due to their high theoretical energy density, low cost and negligible toxicity, Li-air batteries are actively explored as promising energy storage and conversion devices. However, practical use of Li-air batteries is limited in part by sluggish cathode processes, where di-electron O2/Li2O2 chemistry takes place. Due to the low solubility and electronic conductivity of Li2O2, the discharge process suffers from rising impedance that eventually contributes to the "sudden death" of the battery. Similarly, thick Li2O2 deposits cause large charging overpotentials that lower the overall energy efficiency and long-term stability. Here, we address this challenge by investigating soluble redox-mediators and electrocatalysts that promote growth of Li2O2 in the electrolyte solution during discharge and the oxidation of Li2O2 during charge. By driving the reaction away from the electrode surface, we hypothesize that the cell capacity and cyclability of the Li-O2 battery will increase. In addition to redox mediator studies, we are investigating membranes for selective Li-ion transport. Materials for selective membranes are derived from metal organic framework (MOF) motifs, which are known to exhibit excellent tunability of pore size and chemical composition. Our study will result in the development of free-standing MOF membranes with high Li-ion conductivity and efficient separation of the catholyte and anolyte solutions, helping to mitigate the so-called "shuttling effect."

11:00 AM Grafting Synthesis of Silica-Supported Boron (WeA1d)

Melissa Cendejas (University of Wisconsin-Madison), *Rick W. Dorn* (Iowa State University), *Ive Hermans* (University of Wisconsin-Madison), *William P. McDermott* (University of Wisconsin-Madison), *Aaron Rossini* (Iowa State University)

Boron-containing materials have recently arisen as highly selective catalysts for the oxidative dehydrogenation (ODH) of light alkanes to important building block olefins. In the ODH of propane, hBN shows a remarkable 80% propylene selectivity at 8% propane conversion compared to 60% propylene selectivity at 8% propane conversion for the previous state-of-the-art supported vanadium oxide catalysts. ODH over B-based catalysts likely proceeds via a radical mechanism initiated by the surface. An amorphous boron oxide/hydroxide phase has been identified as necessary for catalytic activity. This phase is dynamic under reaction conditions, able to generate metastable boron species, whose predicted catalytic activity can explain the kinetics observed for B-based ODH catalysts. The surface dynamics under reaction conditions and the hypothesized metastable active site mean that ex situ characterization cannot directly observe the active site. Instead, we can use ex situ spectroscopy to probe the requirements for active site formation. In the present study, we attempt to control the extent of boron agglomeration on the fresh catalyst using grafting synthesis. 11B solid state NMR shows that the chemical grafting of pinacolborane to thermally pretreated silica results in isolated monopodal boron species that can hydrogen-bond with neighboring silanol groups. Thermal treatment generates agglomerated boron clusters and nearly identical speciation regardless of boron content or initial speciation. Propane ODH catalytic activity for these materials is typical for silica-supported boron catalysts. Interestingly, these materials exhibit a loss of productivity at higher propane conversions. Detailed kinetic studies are needed to further understand this behavior.

Fluid Properties, Fluid Dynamics, and Transport Phenomena

Wednesday, March 17, 2021 (**WeA2**)
Chair: *Joel Paustian* (Honeywell UOP)
Co-Chair: *Shri Dawande* (Illinois Institute of Technology)

9:45 AM CFD Modeling of a Bioreactor (WeA2a)

Reza Mostofi (Honeywell UOP), *Azita Ahmadzadeh* (Honeywell UOP), *Steve Poklop* (Honeywell UOP)

Computational Fluid Dynamic (CFD) modeling is a powerful tool for equipment design and development and is widely used at UOP, particularly for the multiphase systems. In this application, the hydrodynamic interaction of the air and water in the fixed-bed bioreactor was studied. An innovative and efficient modelling method was incorporated to overcome a complex bioreactor configuration. The critical challenge in this three-phase CFD model was finding an accurate approach to mimic wastewater (hydraulic) and aeration (gas-bubbles) patterns through the solid phase containing substantial biomass. To better understand the flow pattern, flow distribution and the air bubble residence time inside the Bioreactor, the analysis was broken down into two sub-models. Part 1 single-phase water-flow only analysis showed that the packing media caused the water flow to distribute uniformly across the packed-bed, even when high levels of biomass are present, without any channeling or by-pass or plugging. Part 2 two-phase air/water flow analysis showed that the packing void areas affected immediate air flow expansion into and subsequent distribution throughout the high surface area of the packed bed, even with the accumulation of high biomass. This CFD approach was subsequently used for different applications where random or structure packings were to be modeled.

10:10 AM Design of a Fully Integrated Artificial Photosynthetic System for a Moisture-Gradient CO2 Capture and Reduction (WeA2b)

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

The effect of anthropogenic emissions of CO2 on the climate change is becoming progressively prevalent. The current concentration of CO2 in the air is 400 ppm, which is increasing at a rate of ~1.9 ppm per year. There exist several technologies such as amine scrubbing, oxyfuel combustion, and calcium looping to capture CO2 from flue gases, which are inherently energy intensive. However, there are only a few techniques such as moisture-swing adsorption that can capture CO2 from the air but requires modulation of humidity and downstream separation. The captured CO2 can be either sequestered at the storage site or chemically transformed into a usable product. Integrating CO2 capture with reduction not only eliminates the need for additional transportation and storage but also increases the efficiency of CO2 capture. Here we provide a conceptual design and analysis of the transport of species in an integrated system where an anion-exchange resin for CO2 capture is directly connected to a photo/electrochemical cell for CO2 reduction. The CO2 capture in this resin works on a moisture-gradient absorption of CO2 accompanied by a carbonate/bicarbonate equilibrium. The dry-side of the resin captures CO2 from the air and produces a high concentration of HCO3- diffusing towards the wet-side of the resin, where HCO3- converts back to CO2 at the attached cathode to produce fuels. The limiting current density of an integrated system as a function of resin properties, catalysts activity and selectivity, electrolyte pH, physical dimensions and relative humidity are simulated using COMSOL Multiphysics. The limiting current density increases with increasing the resin conductivity, and mass-transfer coefficient of CO2 in air. The efficiency of such integrated system using air as well as flue gas will be discussed as a part of this work.

10:35 AM Maxwell Viscoelasticity of Complex Fluids Mixtures (WeA2c)

Guler Bengusu Tezel (Bolu Abant Izzet Baysal University)

Rheology is a powerful analytical tool for understanding the microstructure and viscoelastic properties of soft matters to obtain more information about the viscoelastic and flow properties of hydrogels based on polymers. The rheological behavior that that is generally investigated incudes constant shear stress or shear rate response, flow behavior under variable shear rate, deformation with increasing oscillatory strain, deformation attributes under variable oscillatory frequency at fixed strain in lineer viscoleastic region. The viscous and elastic properties at low frequency long time scales provide the microstructure including crosslinking polymer chain relaxation informations, while at high frequency short time provide macrostructure information including possible bulk interactions between polymer chains. At short time tests, non-linear viscoleastic characterizations gain importance especially giving viscous contributions and viscosity changings in the bulk fluid. For linear viscoelasticity simulations, Maxwell model can be used to get relaxation times of bulk polymeric systems. This study aims to seek the linear viscoelasticity and relaxation times of different complex fluid mixtures with different mixing concentration, ratio and temperature. Keywords: Rheology; Viscoelasticity; Relaxation times; Maxwell Model

11:00 AM Modeling and Numerical Simulation of Concentrated Solar Energy Storage in a Packed Bed of Silicon Carbide Particles (WeA2d)

Zeyuan Gao (Illinois Institute of Technology), *Javad Abbasian* (Illinois Institute of Technology), *Hamid Arastoopour* (Illinois Institute of Technology)

[**canceled**]

Fluidized bed is considered as a good receiver for concentrated solar power(CSP). In this study, directly irradiated fixed bed and fluidized bed solar absorber under concentrated solar was simulated by CFD technology and the result was compared with experiments. Particles are modelled by Eulerian multiphase model. For conductive heat transfer, heat is transferred by contact area between particles and gas near contact surface. Thus, Zehner-Bauer-Schlünder (ZBS) conductivity model is used to calculate the effective thermal conductivity by thermal conductivity of pure solid and voidage. Radiative heat transfer plays an important role when temperature is high and is modelled as an effective conductivity by Breitbach and Barthels (B-B) correlation. The sub-grid scale model are used for fluidized bed. The result of 2D simulation agree well with thermal measurement by infrared cameral on a directly irradiated fixed bed and fluidized bed solar absorber.

<u>Wednesday Afternoon Keynote Session</u>

Wednesday, March 17, 2021 (**WeK2**)

12:50 PM The Future Ain't What It Used To Be

Cathy Tway (Johnson Matthey)

This famous quote by Yankees legend Yogi Berra seems a fitting description of the predicted changes the chemical economy will undergo. How quickly new feedstocks and energy sources will be adopted is unclear, and yet predictions suggest that moves towards Net Zero and circular solutions are accelerating. This talk will explore a few of those trends and their implications for technology.

<u>Climate Solutions</u>

Wednesday, March 17, 2021 (**WeB1**)

Chair: *Dennis O'Brien* (Jacobs Engineering)

2:00 PM Power, Natural Gas, and the Impacts of Carbon Pricing (WeB1a)

Thomas Rausch (CWE)

Nuclear reactors provide about 20% of all electricity produced in the United States and nuclear generates more carbon-free energy than wind, solar and hydroelectric combined. Since 2013, 11 reactors have closed prematurely and 8 more have announced closure by 2025 or sooner, even though reactor operating costs have been substantially reduced since 2012. Recent power market pricing and generation data of various electric energy sources will be reviewed. The data shows that inexpensive natural gas has resulted in electric market prices that many nuclear owners believe are too low to support continued operation. According to the Nuclear Energy Institute, U.S. reactors prevent production of approximately 500 billion tons of CO_2 per year. This is nearly 10% of the entire carbon dioxide produced in the country annually, from all sources, not just electric generation. Maintaining our nuclear fleet needs to be an important part of any climate policy. Placing a tax or fee on carbon fuels is already being used in many countries as a policy to predictably reduce their fossil fuel use over time. Paired with a border carbon adjustment, it is possible to get enough countries working together so we do not exceed the 1.5° C warming target set by the Intergovernmental Panel on

Climate Change. The presentation will briefly review carbon price legislation already proposed in Congress and discuss how such legislation would impact the competitive positions of the domestic fossil fuel and non-fossil fuel electricity generating mix.

2:25 PM Dispassionate Deliberate Collaboration Can Resolve Global Warming and Its Climate Change Effects (WeB1b)

Thomas Rehm (STS Chair)

Global warming is occurring. It is not a result of a natural cycle. The Arctic is warming three times faster than the planet. There will be massive displacement of populations if we don't figure this out. Solar and wind are all around us. Many say we only need to capture the vast solar energy that strikes the planet. These thoughts are dripping with passion. Passion is invigorating but is it helpful? Movement on important policies depends in great part on advocacy driven by public passion. Some societal issues, perhaps many, can be resolved on the momentum of public passion and resultant political interests to assuage that passion. Global warming and its climate change effects are a different animal. We must be dispassionate. We must be deliberate. We must collaborate. We cannot get this wrong

2:50 PM Clues to Climate Mitigation Priorities from Global Greenhouse Gas Budgets (WeB1c)

Gavin McNicol (University of Illinois at Chicago), *Max Berkelhammer* (University of Illinois at Chicago)

The role of rising atmospheric carbon dioxide, methane, and nitrous oxide in contemporary climate change is now incontrovertible, however, knowledge of global sources and sinks of these three main greenhouse gases is still far from complete. Global greenhouse gas budgets, such as those spearheaded by the Global Carbon Project, combine Earth system modeling, knowledge of global biogeochemical cycles, and economic inventory data (energy production, land conversion, and other activities) to provide a comprehensive overview of climate forcing emissions. These inventories are critical for assessing what the most effective solutions are to reduce emissions and also audit the success of ongoing efforts. This presentation will: 1) briefly describe the top-down and bottom-up methodologies that are both used to create the greenhouse gas emission budgets; 2) review the key insights gained from the most recent global carbon dioxide (2019), and methane and nitrous oxide (2020) budgets, with particular attention to the largest emissions sources and sinks, and their geographic distribution and current trajectories, including COVID-19 pandemic effects; and 3) conclude with discussion of some recently proposed greenhouse gas mitigation opportunities.

<u>**Energy Storage I**</u>

Wednesday, March 17, 2021 (**WeB2**)

Chair: *Hakim Iddir* (Argonne National Laboratory)

Co-Chair: *Juan Garcia* (Argonne National Laboratory)

2:00 PM Strain-Driven Surface Reconstruction and Cation Segregation in Layered Li(Ni1-x-yMnxCoy)O2 (NMC) Cathode Materials (WeB2a)

Juan Garcia (Argonne National Laboratory)

The composition, structure and phase transformations occurring on cathode surfaces greatly affect the performance of Li-ion batteries. Li-ion diffusion and surface-electrolyte interaction are two major phenomena that impact the capacity and cell impedance. The effects of surface reconstruction (SR) of cathode materials on the performance of Li-ion batteries are of current interest. However, the origin and evolution of the SR are still not well understood. In this work, Density Functional Theory (DFT) calculations are used to investigate the processes taking place during surface segregation and reconstruction. Facet dependent segregation was found in Li(Ni1-x-yMnxCoy)O2 (NMC) cathodes. Specifically, Co tends to segregate to the (104) surface of the primary particles within the transition metal layer, while Ni ions tend to segregate to the (012) surface in the Li layer, forming a SR. Experimental evidence shows the SR to be epitaxial with the bulk of the as-synthesized material, the new SR phase is pinned to the NMC unit cell leading to a strained SR. Here, we show that strain can stabilize a spinel structure of the SR layers. Understanding the effects of surface strain opens a new avenue for the design of cathode materials with enhanced surface properties.

2:25 PM Structure-Activity Relationships in Lithium Ion Batteries: Solid State NMR Characterization of Lithium-Ion Cathodes and Anodes (WeB2b)

Fulya Dogan (Argonne National Laboratory)

Strategies for developing new chemistries for lithium ion battery systems with higher energy density, stability and safety involve understanding and mitigating the problems of existing materials through understanding the structural changes and their relations with materials activity. This can largely be achieved with detailed structural characterizations of the active battery materials. For lithium ion cathodes, some of the mitigation strategies involve, increase of lithium content, change transition metal composition and use of different dopants and surface coatings. However, each change brings additional challenge to understand the structural modifications induced and its relationship with materials activity. For lithium ion anodes, recent efforts focus on replacing the traditional graphite anode with higher capacity materials such as the silicon. This talk will focus on the application of multinuclear solid-state NMR spectroscopy as a structural probe on lithium ion cathodes and anodes. On cathode side, we will look at the evolution of surface, interface and bulk of cathodes with different synthesis conditions and electrochemical cycling. On the anode side, we will focus on silicon electrodes and examine the electrode-electrolyte interaction and SEI formation processes to study new electrolyte systems that can be used in future silicon-based anodes for Li-ion batteries. These characterization efforts not only provide insights and understanding on how electrode structure effects activity and evolves during electrochemical cycling but also guide material development and synthesis efforts to design improved electrodes.

2:50 PM Understanding the (de)Lithiation Mechanism of Pb-Based Nanocomposite Anode for High Performance Lithium-Ion Batteries (WeB2c)

Jinhyup Han (Argonne National Laboratory), *Seong-Min Bak* (Brookhaven National Laboratory), *Jihyeon Gim* (Argonne National Laboratory), *Xiaobing Hu* (Northwestern University), *Christopher Johnson* (Argonne National Laboratory), *Youngsik Kim* (Ulsan National Institute of Science and Technology), *Eungje Lee* (Argonne National Laboratory), *Jehee Park* (Argonne National Laboratory), *Seoung-Bum Son* (Argonne National Laboratory), *Chi Cheung Su* (Argonne National Laboratory), *Cesar Villa* (Northwestern University)

A high-energy ball milling method was used to prepare a lead oxide (PbO) shell on core of lead (Pb) nanoparticles. The resultant composite Pb@PbO-C results in excellent Li-ion cell electrochemical properties of ~600 mAh/g reversible (de)lithiation capacities with a retention of 92% over 100 cycles. This value represents a step improvement over previous studies in the lead system. It is attributed to the self-limiting process of oxidation of Pb nanoparticles to PbO composite thus maintaining a nanostructured material sufficient for good electrochemistry. This process is simple and uses low-cost precursors of lead oxide and carbon. Furthermore, the detail mechanism of Li-Pb alloying and dealloying reaction was investigated by conducting operando synchrotron X-ray diffraction and ex-situ X-ray absorption spectroscopy analytical methods. The characterization results show that the Li-Pb binary alloy phase diagram is followed, and the electronic nature of the (de)lithiation of the process is attributed to Li to Pb charge transfer in a Zintl-type phase.

<u>Biorefining Technology</u>

Wednesday, March 17, 2021 (**WeC1**)

Chair: *Belma Demirel* (BP)

3:45 PM The Pursuit of a Cleaner Healthier World through Bio Renewables (WeC1a)

Grace Rhoades (Johnson Matthey)

The growing concern over climate change has created a push in the fuels and chemicals industry to replace petroleum feedstocks with bio-based alternatives. Traditionally bio-based feedstocks have referred to energy crops like corn starch or soybean oil for ethanol and biodiesel production. However, recent technical developments and added incentives to use lower carbon feedstocks have led to the rise in production of advanced biofuels. This includes the expansion of renewable diesel and bio-jet fuel production from more sustainable feedstocks such as Used Cooking Oil (UCO) and Municipal Solid Waste (MSW). Added incentives from the government and an eco-conscious consumer base are driving the transition to produce more biofuels and biochemicals. For biofuels the primary driver is legislation that provides credits to replace fossil-based transportation fuels with lower carbon alternatives. Future policy is expected to focus on the sectors that are hardest to decarbonize which include long-haul trucking, and long-distance aviation. In contrast, the biochemicals market is primarily pulled by consumer demand for sustainable products. Plastics and packaging are generating the most attention because this is the largest petrochemical sector and single use plastic contributes the most to pollution and marine debris. Johnson Matthey is currently engaged in a variety of biofuel and biochemical operations. These technologies have been developed with leading industry partners in our pursuit of a cleaner healthier world. Of these three current projects will be highlighted.

4:10 PM Techno-Economic Analysis of the Modified Mixalco Process (WeC1b)

Chloe Simchick (Milwaukee School of Engineering) [**canceled**]

The MixAlco process is a patented biomass conversion technology which relies on the use of fermentation to convert a variety of biomass into useful chemicals. Unlike previous MixAlco designs which model the production of hydrocarbon fuels, this proposed design simulates mixed carboxylic acid production. These have a more competitive selling price than hydrocarbon fuels. For the base case feed rate of 18.5 US tons of biomass per hour, the estimated total capital investment is $28,949,000, and the payback time at a 47.54% ROI is 2.10 years at a minimum selling price range of $1.90-$2.38 per gallon. Sensitivity analysis identified four critical input factors of the process: biomass feed rate, selling price, distribution cost, and biomass composition. Overall, the sensitivity analysis of all four input factors support that the new design is flexible in its ability to support populations of varying sizes as well as different biomass feed rates and compositions.

4:35 PM OPEN (WeC1c)

<u>Energy Storage II</u>

Wednesday, March 17, 2021 (**WeC2**)

Chair: *Juan Garcia* (Argonne National Laboratory)

Co-chair: *Hakim Iddir* (Argonne National Laboratory)

3:45 PM A Lithium Accounting Model with Unstable Electrolytes: Protocol Dependence, Invisible Processes, and the Consequences of Reactivity (WeC2a)

Adam Tornheim (Argonne National Laboratory)*, Daniel O'Hanlon* (Argonne National Laboratory)

A lithium inventory model is presented in which battery performance metrics of capacity retention (CR) and Coulombic efficiency (CE) are derived in terms of side-reaction rates at each electrode surface (oxidation at the cathode, reduction at the anode). The model indicates that CR and CE depend strongly on cycling rate and side-reaction rates in a manner that differs depending on the anode's lithiation state following discharge. The model provides a method for calculating side-reaction rates from CR and CE. Experimental results are presented to support the model along with calculated side-reaction rates at each electrode for a nickel-rich layered oxide/graphite system.

4:10 PM NiMn5050-Based Cathodes As Next Generation Cathodes for Lithium-Ion Battery (WeC2b)

Anh Vu (Argonne National Laboratory), *Jason Croy* (University of Central Florida)*, Yang Ren* (Argonne National Laboratory)

Cathode materials with low or no cobalt have been attracting great attention as the next generation cathodes for lithium-ion batteries in efforts to reduce security critical materials. Mn0.5Ni0.5-based cathodes are strong candidates to replace Co-based cathodes due to the synergetic combination of Ni2+ and Mn4+, which Ni2+ can be fully oxidized to Ni4+ to realize high capacity and Mn ions remain as Mn4+ providing the structural stability during the operation. The challenge with reducing cobalt in LiMnxNiyCo1-x-yO2 cathodes is an increased propensity for Li-Ni mixing, which blocks the diffusion of Li ions, thereby lowering the capacity and hindering the high-rate performance of these materials. In this study, we investigated a series of Mn0.5Ni0.5-based cathodes synthesized under different synthesis conditions to elucidate the effects of Ni, Mn, and Co on the structures as well the echem performances of these cathodes. In-situ XRD was used to study the thermal behaviors of selected Co-free and low-Co containing Mn0.5Ni0.5-based cathodes to understand how the temperatures and the heating-cooling rates affect the structure of these cathodes. Our studies showed that local minima in the Li-Ni exchange occurred under different conditions for Co-free and for low-Co containing Mn0.5Ni0.5-based cathodes. The results help guild the design and the synthesis of low-cobalt materials in order to have better control over Li-Ni exchange and the associated electrochemical properties of the final cathode products.

4:35 PM Lead-Based Nanocomposites As Anode Material for Sodium-Ion Batteries (WeC2c)

Jehee Park (Argonne National Laboratory)*, Shabbir Ahmed* (Argonne National Laboratory), *Seong-Min Bak* (Brookhaven National Laboratory), *Jihyeon Gim* (Argonne National Laboratory), *Jinhyup Han* (Argonne National Laboratory), *Christopher Johnson* (Argonne National Laboratory), *Youngsik Kim* (Ulsan National Institute of Science and Technology), *Eungje Lee* (Argonne National Laboratory)

Sodium ion batteries (SIBs) have attracted much attention as alternative to Lithium ion batteries due to abundant sodium source and comparatively low cost [1]. Anode materials using conversion and alloying reactions have been studied for high energy density of sodium ion batteries. Among many candidates, lead-based materials such as lead (Pb) and lead oxide (PbO) have advantages of low cost and high volumetric capacity. Despite their potential for new anode for SIBs, the lead-based materials have received little attention due to their toxicity issue. However, lead has been one of the most recycled materials with a high global recycling rate of 99 % in the United States [3]. Also, when Pb is used as anode with sodium layered cathode, the energy density of pouch type cell is 549 Wh/L and cost is lower than 63.5 USD/kWh according to Argonne BatPac model [4]. Therefore, Pb-based materials have competitive potential as promising anode for low cost and high energy SIBs. In this work, we present novel Pb-based nanocomposite synthesized by high energy milling method using carbon matrix. Electrochemical data show high capacity of 381 mAh/g and good cycle performance for 50 cycles with capacity degradation of 27%. Reaction mechanism will be demonstrated by synchrotron X-ray characterization. Also we suggest intermetallic Pb-M (M = Sn, Sb, Fe, Mn, Ni) composite materials using active/inactive and conductive matrix for development. [1] Journal of The Electrochemical Society, 2015, 162 (14) A2538-A2550 [2] Sustainable Materials and Technologies, 2014, 1-2, 2-7. [3] BatPaC, Argonne National Laboratory. (n.d.). http://www.cse.anl.gov/batpac.

Local Section Dinner and Dinner Keynote

Wednesday, March 17, 2021 (**WeK3**)

6:00 PM Using Molecular Modeling for Screening and Optimizing Membrane Based Separation Processes

Sohail Murad (Illinois Institute of Technology)

Separations consume almost 15% of the total global energy consumption. These separations ae currently almost exclusively thermal. Membrane based separations offer a energy efficient alternative, but the development of these methods has been challenging. One possibility to address these challenges is to use computational tools for screening design alternatives rather than using traditional engineering techniques for lab scale to commercial designs. We will describe how molecular simulations using a method based on molecular dynamics can be used to study and design a wide variety of separation processes. These include reverse osmosis separation of brine, separation of air and N2-CO2 mixtures using zeolite membranes, pervaporation separation of alcohols, and selective permeation of heavy ions and protons in ion exchange membranes used in the new generation of redox batteries. Finally molecular simulations have been used to understand anomalous behavior observed in experimental studies

Presentation Abstracts

Thursday, March 18, 2021

Thursday Morning Keynote Session
Thursday, March 18, 2021 (**ThK1**)

8:40 AM Science and Society
Marius Stan (Argonne National Laboratory)

Elements of science, engineering, and technology have positively impacted human society throughout history. Among the most spectacular developments are the discovery and design of new materials and chemical compounds. With the volume, variety and rate of data generation continuously increasing, human analysis becomes extremely difficult, if not impossible. In this talk, the concept of "intelligent software" is introduced and discussed. The software includes elements of Artificial Intelligence such as machine learning and computer vision, coupled with reduced-order modeling and Bayesian statistics for uncertainty evaluation. The value of the approach is illustrated using examples of material design and real-time optimization of synthesis processes. The presentation also includes a discussion of the impact of AI and computational science on society, with a focus on lifestyle, cinema, and visual arts.

Machine Learning and Optimization
Thursday, March 18, 2021 (**ThA1**)
Chair: *Joshua Gabriel* (Argonne National Laboratory)
Co-Chair: *Aditya Prajapati* (University of Illinois at Chicago)

9:45 AM Machine Learning Force Fields for Li-Ion Cathodes (ThA1a)
Joshua Gabriel (Argonne National Laboratory), *Juan Garcia* (Argonne National Laboratory), *Hakim Iddir* (Argonne National Laboratory), *John Low* (Argonne National Laboratory), *Noah Paulson* (Argonne National Laboratory), *Marius Stan* (Argonne National Laboratory)

Machine Learning Force Fields (MLFF) have emerged as a tool to accelerate the atomic scale modeling of materials while preserving accuracy of density functional theory calculations. A workflow for developing such an MLFF, which leverages state of the art deep learning high performance computing architectures available at the national laboratories, is presented and discussed. The MLFF is used to study the thermodynamics and structural changes of lithium nickel oxide (LNO) battery cathode material during room temperature operation. The results emphasize the complexity of phase stability in this system and demonstrate the predictive power of the MLFF method.

10:10 AM Cost Productivity Approach to Industry 4.0 Cybersecurity (ThA1b)
Pranav Patel (ResiliAnt by MediTechSafe)*, Prerak Patel* (ResiliAnt)

Cyber-physical systems with Internet of Things (IoT), Big Data and Cloud Computing in Industry 4.0 promises to deliver improved productivity, quality, and compliance. According to experts, increased interconnectedness and digital collaboration across a supply-chain can further reduce operational costs by at least 30% and reduce inventory requirements by as much as 70%. The exponentially increasing connectivity, however, raises concerns around cybersecurity; more connected Things means an expanded attack surface for hackers. Many studies have demonstrated that up to 80% of connected devices or equipment in a plant tend to have security vulnerabilities. Ransomware events such as the ones faced by Norsk Hydro, Hexion, X-fab, TSMC, Luxottica, Honda and Momentive cause considerable operational disruption and serve as a warning to all organizations. In fact, a forced shut down of a gas compression facility earlier in 2020 due to a cyber-attack as well as a ransomware attack faced by a US Maritime base that brought cameras, door-access control systems, and critical monitoring system down for 30 hours serves as a reminder of growing cyber-threats. This year, hackers exploited remote access to SCADA to increase sodium hydroxide levels by more than 100x in a water treatment plant in Florida. In this session, attendees will gain understanding of how to best to take an ROI-minded risk-based approach to OT/IoT cybersecurity. The session will also cover an easy-to-use and quickly implementable approach that can help address 4x more risk while delivering up to 70% cost productivity.

10:35 AM Artificial Intelligence (AI) – Machine Learning (ML) Based Framework for Optimal Design of Interfacially Polymerized Thin Film Nanocomposite Membranes for Desalination (ThA1c)
Jasneet Kaur Pala (BITS Pilani K K Birla Goa Campus)
[**canceled**]

Introduction to Machine learning and Artificial Intelligence in the Chemical engineering field has brought an immense positive impact in handling complex data and for better visualization. The current work focuses on the AI-ML framework for the design of optimal thin film nanocomposite membrane and operating parameters for yielding the best performance in terms of permeability and salt rejection capabilities. A total of 315 data points were reviewed classified into various operating as well as membrane synthesis parameters including polymer, solvents, temperature, thin film composite layer formation, and nanoparticle properties. These data underwent comparative analysis using 6 AI-ML based models like Multi Linear Regression (MLR), Ridge Regression (RR), Random Forest Regression tree (RFRT), Gaussian Process Regression (GPR), Gradient Boosting Regression Tree (GBRT), and Artificial Neural Network (ANN). These models were compared on basis of their performance criteria like R2 and RMSE values on basis of their water permeability and salt rejection predictions. It was found that MLR / RR were the worst performing models and ANN predicted the data most accurately (R2>0.98). Further Single Objective Optimization (SOO) and Multi-Objective Optimization (MOO) were carried out to determine the optimal TFN composition and operating conditions using the ANN model. The best solutions are identified where both permeability and salt rejections were > 85 l/m2.h and salt rejection > 99% and they were (i) nanoparticle weight % 0.0087-0.27 wt%, (ii) optimum pressure = 14 – 31 bar, (iii) feed temperature = 45 – 52 oC for (iv)11,000 ppm NaCl feed solution.

<u>Process Safety and Occupational Health I</u>

Thursday, March 18, 2021 (**ThA2**)
Chair: *David Hietala* (Exponent)
Co-Chair: *Jessica Morris* (Exponent)

9:45 AM Why Storage Tanks Leak and How to Stay Safe (ThA2a)
Jessica Morris (Exponent), *Ryan Hart* (Exponent), *Delmar Morrison* (Exponent)

Atmospheric and low pressure storage tanks are necessary for storing bulk liquid chemicals in chemical manufacturing process facilities. When these storage tanks are filled or undergo changes in temperature, pressure, or composition that exceeds its specified storage conditions, they have the potential to vent and release some of their contents. When a tank vents a flammable vapor, the event can lead to potential hazards such as a fire or explosion. Causes of overpressure or vacuum, venting requirements, and venting devices will be discussed with respect to API RP 2000 - Guide for Venting Atmospheric and Low-Pressure Storage Tanks. Modeling of different venting scenarios in Phast (Process Hazard Analysis Software) will be utilized for aid in discussion.

10:10 AM Mechanical Integrity for Aging Process Facilities - Ensuring Safe Operations over Time (ThA2b)
Robert Weber (PSRG Inc.)

Aging equipment and facilities is a process safety and risk management challenge. Aging infrastructure can increase the frequency and severity of equipment failure. A recent FM Global study showed 50% of major hazard loss of containment events were a result of failures primarily due to aging mechanisms, such as erosion, corrosion and fatigue. Another 2013 study by the U.S. Chemical Safety Board found that inadequate mechanical integrity programs, delayed or deferred maintenance, and aging infrastructure of equipment at industrial facilities was a recurring root cause of incidents. In order to effectively manage aging assets, a proactive strategy is required before a failure occurs. This paper introduces methods to help managers and supervisors make better risk-based decisions and develop a robust maintenance strategy to deal with aging equipment and infrastructure as it approaches the end of its lifecycle.

10:35 AM Combustible Dust Hazards and Spray Drying Systems – Understanding NFPA 61's New Requirements in a Dust Hazard Analysis (ThA2c)
Sean Dee (Exponent), *Brenton Cox* (Exponent), *Russell Ogle* (Exponent), *Matthew Walters* (Exponent)

NFPA 61 - Standard for the Prevention of Fires and Dust Explosion in Agricultural and Food Processing Facilities was first issued in 1995 and continues to be the primary combustible dust standard for agricultural and food processing facilities. The current edition of NFPA 61 was approved in late 2019 and several changes were made to align NFPA 61 with NFPA 652 – Standard on the Fundamentals of Combustible Dust. NFPA 652 was developed in the 2010s and first issued as a 2016 edition. NFPA 652 is a broader standard that applies to a variety of industries that handle combustible dust. Specifically, NFPA 652 includes provisions for conducting dust hazard analyses for new and existing processes in an effort to improve the identification and mitigation of combustible dust hazards. The current edition of NFPA 61 added new requirements for Spray Drying Systems, which are now included as a subcategory of dryer in NFPA 61's equipment section. These new requirements lay out approaches for managing combustible dust hazards in spray drying systems and their interconnected equipment. This presentation will provide an overview of spray drying systems in food and agricultural facilities, review the new requirements for spray drying systems in NFPA 61, and discuss how these new requirements play a role in a dust hazard analysis (DHA) that may be conducted on spray drying systems in accordance with NFPA 652. Finally, an example case study DHA for a spray drying system will be presented to illustrate the concepts outlined in NFPA 61.

Thursday Afternoon Keynote Session
Thursday, March 18, 2021 (**ThK2**)

12:50 PM Process Safety Update - Training, Research, ... Where Are We Headed?
Ray Mentzer (Purdue University)

Following the T2 Laboratory incident in FL in 2007, all ABET accredited Chemical Engineering curricula have been required to address process safety. Numerous approaches, with only a few schools choosing to require a rigorous technical course, but number seems to be growing – albeit, slowly. What does such training generally consist of and what are the challenges academics have in offering such training? The Davidson School of Chemical Engineering at Purdue University is deeply committed to process safety and requires such rigorous training for all seniors. In addition, the *Purdue Process Safety & Assurance Center* (P2SAC) was formed in 2014 focused on process safety research at the PhD, MS and undergraduate levels. Projects are suggested by industry sponsors who represent a broad spectrum of industries – oil & gas, chemicals, pharmaceuticals, manufacturing, etc – many of whom serve as mentors during the work. Several recent projects will be highlighted, including a snapshot of the future direction & challenges in this technical multifaceted discipline.

Advances in Refining
Thursday, March 18, 2021 (**ThB1**)
Chair: *Belma Demirel* (BP)
Co-chair: *Shahineze Saada* (Honeywell UOP)

2:00 PM Reducing Octane Loss – Solutions for FCC Gasoline Post-Treatment Services (ThB1a)
Claus Brostrom Nielsen (Haldor Topsoe A/S)

As sulfur regulations tighten, refiners find it increasingly difficult to meet specifications from their FCC gasoline post-treatment units. The octane number, especially, suffers because of the necessary sulfur removal. Understanding the feedstock chemistry can lessen the octane loss and the overall impact on the refinery economics. This presentation will describe the levers available to the refinery to reduce the octane loss. We will take you through the chemical reactions taking place in any FCC gasoline post-treatment unit. We will also illustrate how the unit layout and each hydroprocessing section in the unit play an important role in meeting the sulfur specifications and how they contribute to the overall octane number. The presentation will also highlight how the different types of catalysts can contribute to meeting the 10 wtppm product sulfur requirements, including the new Topsoe HyOctane™ FCC gasoline post-treatment catalysts, and why specially developed catalysts with high selectivity is needed. We will show how the combination of feedstock chemistry, unit layout, and specially developed catalysts will provide the optimal solution for FCC gasoline post-treatment and meet the product requirements of ultra-low gasoline and low octane loss.

2:25 PM Premium Performance Delivered in Challenging Middle Distillates Hydrotreating Operations
(ThB1b)

Aaron Joss (Albemarle)

Over the last years, new Hydrotreating catalysts have been introduced in the market primarily to serve operations with high pressure and hydrogen availability. Catalyst innovation for operations limited by hydrogen, such as low and medium pressure Middle Distillates-HydroTreating (MD-HT) on the other hand, has been significantly slower and less groundbreaking. The challenge was being able to design premium catalyst solutions that could offer better performance with limited hydrogen supply while still guaranteeing high flexibility in feed diet and stability over the entire operating cycle. To improve stability for hydrogen constrained MD-HT operations, suppliers mainly sought to develop moderately active catalyst systems. The consequence was that, while benefitting from the stability of these catalysts, refiners were not able to extract the full operating potential and profit from their critical Hydrotreating units. Continued research at Albemarle has now led to the introduction of a new superior class of catalysts, PULSAR™. PULSAR catalysts are based on a breakthrough design that combines optimization of the morphology of the support as well as of the metal active phase. The result is significantly higher activity per reactor volume at increased stability, even in operations limited by hydrogen availability. Albemarle's new premium catalyst for low and medium pressure, KF 787 PULSAR will be introduced, featuring evidence of its distinctive properties and performance, and discussing the advantages it provides to refiners in practice.

2:50 PM Ultra-High Temperature Resistant Preformed Particle Gels for Enhanced Oil Recovery (ThB1c)

Buddhabhushan Salunkhe (Missouri University of Science and Technology), *Baojun Bai* (Missouri University of Science and Technology), *Thomas Schuman* (Missouri University of Science and Technology)

Gel treatment is one of the most efficient enhanced oil recovery techniques used for conformance control. In recent years, preformed particle gels (PPG) have gained attention for conformance control and to reduce water production. However, there are no current products available to withstand reservoir conditions with high temperature, high pressure, and high salinity. In this paper, we describe the development, characterization and detailed evaluation of a unique hydrogel composition with ultrahigh temperature resistance (HT-PPGs) for chemical enhanced oil recovery. HT-PPG described herein can swell more than 30 times its initial volume in brines of different ionic strengths. We systematically evaluated the effect of variables like temperature, pH, salinity, monovalent vs divalent ions on swelling behavior. The HT-PPGs are mechanically robust in nature with storage moduli (G') of over 3000 Pa at about 90 percent water in content. Additionally, HT-PPGs showed excellent thermal stability at 150 °C for more than 12 months in monovalent and divalent ion containing brines at all swelling ratios. HT-PPGs exhibit exceptional hydrolytic thermal stability for more than 18 months in 2% KCl brine (at water content of > 93 percent) at 150 °C. Coreflooding test was performed in a fractured core and showed good plugging efficiency, helped to reduce the permeability of fracture and did not wash out during the test. HT-PPG discussed in this work, is a unique product with excellent features which make it an ideal candidate for conformance control of reservoirs with harsh temperature, salinity conditions.

Process Safety and Occupational Health II

Thursday, March 18, 2021 (**ThB2**)
Chair: *Jessica Morris* (Exponent)
Co-chair: *David Hietala* (Exponent)

2:00 PM Understanding Fire Hazards in Inert Cryogenic Systems (ThB2a)

Ehson Fawad Nasir (Exponent), *Sean Dee* (Exponent), *Suzanne Smyth* (Exponent), *Nicholas A. Traina* (Exponent)

In the food and agricultural industry, cryogenic refrigeration using liquid nitrogen offers many advantages compared to other refrigeration systems. Liquid nitrogen has a very low boiling point, is chemically inert, and has a high cooling capacity. Many are familiar with the asphyxiation and cold burn hazards posed by liquid nitrogen and some detailed references also address the explosion hazard posed by the rapid vapor expansion of liquid nitrogen in a closed system. However, the factors that make liquid nitrogen an excellent candidate for a cooling fluid (low boiling point, and inert atmosphere) also cause many to overlook the potential fire hazards posed by cryogenic liquid nitrogen systems. These systems operate at temperatures that are sufficiently cold to condense air, potentially resulting in fire hazards posed by liquid oxygen enrichment. Mitigative controls for asphyxiation hazards, such as forced ventilation with air, may also further exacerbate the fire hazard. This presentation will review the characteristics of liquid nitrogen that contribute to both the commonly identified hazards, and the lesser known fire hazard. Good practices for handling liquid nitrogen and systems where liquid oxygen formation may occur will be reviewed. Demonstrative experiments will be presented that illustrate the hazards posed by condensed air that can form in cryogenic systems. Finally, a hypothetical case study will be presented that illustrates the fire hazard posed in these systems, and how users can identify and mitigate such hazards in their cryogenic liquid nitrogen system.

2:25 PM Common Cause Failure – What Are They and How to Mitigate Them? (ThB2b)
Tekin Kunt (PSRG Inc.)

Hazard control and mitigation often relies on multiple safeguards. Usually we build redundancy into our safety systems to make them more robust and responsive. However common cause failures either due to an instantaneous event such as flooding or due to prolonged deviations in the process such as vibrations make these safeguards ineffective simultaneously. In this talk, we will define common cause failures and explore their underlying causes such as the root cause and the coupling factor. At the end of the talk, attendees will be able to identify blind spots in their safety systems.

2:50 PM Means to Achieve Backflow Prevention of Hazardous Chemicals from Process Vessels to Utility Pipelines (ThB2c)
Deepak Sharma (Bayer US)

Design of a chemical manufacturing facility is a challenging task because one has to ensure that every design feature has been carefully analyzed for Hazard and Operability (HAZOP). Along with the HAZOP studies of the main process components like reactors, crystallizers, distillation columns, etc., it is imperative to study the possible failures of the utility connections, which may get overlooked. A system is as safe as its weakest point of failure. A common failure is the back flow of hazardous chemicals into the utility connections. Utilities like nitrogen, steam, plant air, and deionized water are often directly connected to process vessels. The utility systems are generally common to the entire plant and so depending on the reaction conditions in an equipment, backflow may occur and contaminate other equipment. Different backflow prevention instrumentation is required based on the utility service. For instance, gaseous and liquid utilities require different backflow preventors. While choosing the material of construction of pipelines, specification brakes are placed at junctions where utilities are connected to the process vessels. This talk will outline various backflow preventor setups that have been successfully implemented in different chemical manufacturing facilities. Based on the severity of failure, the back flow prevention appropriate for different utility services will be discussed. Different kinds of back flow preventors, including differential pressure measuring instruments, flow transmitters, liquid trap with level switch, on/off valve with interlock activation etc., will be explained in detail and compared for their function and safety features.

<u>**Environmental Compliance and Remediation**</u>
Thursday, March 18, 2021 (**ThC1**)
Chair: *Jarad Champion* (Geosyntec)

3:45 PM Destructive Technologies for per- and Polyfluoroalkyl Substances (PFAS) (ThC1a)
Mary Ensch (Geosyntec)

Per- and polyfluoroalkyl substances (PFAS) are emerging contaminants that have toxic health effects. Due to their wide-spread presence in the environment and inability to degrade, they require remediation. Currently, remediation methods that are implemented are mass transfer processes. These may include excavation and disposal for solids, and adsorption or filtration methods for liquids. These technologies do not destroy the PFAS in the contaminated matrix but transfer them to either a landfill, media such as granular activated carbon (GAC) or anion exchange resins (IX), or into a concentrated waste stream. The primarily known and used destruction technology for PFAS is incineration. However, there are knowledge gaps surrounding the generation of byproducts with this technology, or its ability to achieve complete combustion of all PFAS. Due to the increasing need for destructive technologies, university laboratories have begun investigation into alternatives. These up-and-coming technologies include electrochemical oxidation, heat activated persulfate oxidation, ozone oxidation, smoldering, and plasma defluorination. This presentation will describe the state of development of each technology with a primary focus on electrochemical oxidation.

4:10 PM Improving Membrane Fouling Resistance in Water Filtration with Polyelectrolyte Complex Sacrificial Layers (ThC1b)

Yechan Wong (Geosyntec)

The improvement of fouling control in water filtration processes promotes optimum membrane performance and can reduce capital, and operations and maintenance costs. A polyelectrolyte complex (PEC) sacrificial layer casted on a ceramic membrane via salt induced phase inversion was prepared and functionalized with negatively charged carboxymethyl chitosan (CMC−) and positively charged quaternized chitosan (QC+) to achieve membrane fouling resistance. The CMC− functionalized PEC (CMC−/PEC) and QC+ functionalized PEC (QC+/PEC) were evaluated for their surface charge, antibacterial action against Pseudomonas putida, and flux decline and recovery using a synthetic feed solution. CMC−/PEC and QC+/PEC exhibited charge-based, selective repulsion of model organic and inorganic substances and displayed lower bacterial attachment and higher bactericidal activity compared to those of a bare ceramic membrane. In fact, the ceramic membrane was negligibly bactericidal whereas CMC−/PEC and QC+/PEC had cell viability of 34.4 ± 10.2% and 30.6 ± 8.2%, respectively. Among the PEC samples, CMC−/PEC had the lowest cell attachment while QC+/PEC had the highest cell attachment because of electrostatic interactions between Pseudomonas putida and the PEC surfaces. In the flux decline and recovery experiments, the PEC samples showed lower rates of flux decline due to organic fouling than did the bare ceramic membrane and promoted much higher flux recoveries through removal and reestablishment of the PEC sacrificial layer than simply backwashing the bare ceramic membranes after fouling has occurred. The PEC opens a new possibility of effective membrane fouling control through surface functionalization and creation of sacrificial layer for an underlying membrane.

4:35 PM Are Catastrophes Affecting Compliance? (ThC1c)

Katherine Culbert (K and K Process)

Industrial processes are under constant review from various regulatory bodies, whether Local, State, or Federal, and catastrophic events have an impact on operations and reporting requirements. In this session, we will review events in the "Energy Capital of the World," and look at how compliance activities are impacted. Hurricane Harvey wreaked havoc on the Houston area in 2017 with unprecedented rainfall which flooded the entire area and Texas Governor Abbott suspended numerous rules regarding pollution control equipment and operations at industrial facilities. The flooding caused, among other things, Arkema's chemical manufacturing refrigeration system to fail, resulting in a fire and explosion of organic peroxides. In 2019, the Intercontinental Terminals Company experienced a fire that blazed for days and sent a thick black plume of smoke over the area and chemical releases into nearby waterways. The fire resulted in an uncontained release of Naphtha enriched with Butane. The fire response affected the Houston Ship Channel and Galveston Bay with water runoff in addition to the tank leakage that allowed thousands of barrels of material into the waterways. And this year, the state of Texas saw low temperatures it has not seen in over 30 years, causing a catastrophic failure of the electrical grid. It is still being determined what the environmental impact will be from the fallout.

<u>Biomedical, Pharmaceutical, and Nano-Engineering</u>

Thursday, March 18, 2021 (**ThC2**)

Chair: *Abhinav Bhushan* (Illinois Institute of Technology)

Co-chair: *Seok Hoon Hong* (Illinois Institute of Technology)

3:45 PM Polymersome Encapsulation of a High Logp Protein-Protein Interaction Inhibitor to Achieve Increased Solubility and Therapeutic Index (ThC2a)

Yu Tian (University of Delaware), *James L. LaBelle* (University of Chicago), *Mathew R. Schnorenberg* (University of Chicago), *Matthew V. Tirrell* (University of Chicago)

Protein-protein interactions (PPIs) dictate most biological processes, including those responsible for carcinogenesis. Targeted therapeutics acting on these oncogenic PPIs are the focus of novel drug discovery. Currently,one small molecule PPI inhibitor, Venetoclax is FDA approved to treat a number of hematologic malignancies through its inhibition of BCL-2. However, considering that there are ~650,000 potential human PPI targets, the development of other PPI inhibiting drugs has been lagging due to the off-target and delivery issues. For example, ABT-263 although possessing potent nanomolar binding affinity to BCL-2, can lead to sever thrombocytopenia due to the off-target BCL-XL inhibition in platelets. This is limiting its therapeutic index. We have developed a nanocarrier system, targeted polymersome (PSOM) nanoparticle, made of poly(ethylene glycol)-disulfide-poly(propylene sulfide) (PEG-SS-PPS) with surface conjugated anti-CD19 F(ab) antibody fragments (αCD19Fabs) as targeting motif to B cell lymphoma. PSOMs are fabricated by flash nanoprecipitation (FNP) and extrusion resulting in uniform vesicular morphology and size distribution (~130 nm in diameter). Moreover, ABT-263 was successfully encapsulated by PSOM at an efficiency over 90%, which increases the solubility of the lipophilic ABT-263 to over 10mM in PBS. From in vivo platelet-counting, the intravenous administration of PSOM encapsulated ABT-263, in contrast to orally administered non-encapsulated drug, led to the mitigated thrombocytopenia in mice. Importantly, flow cytometric analyses on a panel of human CD19 positive diffuse large B cell lymphoma cell lines demonstrated specific uptake of αCD19-PSOM nanoparticles. We believe the results indicate the promise of in vivo targeted delivery of ABT-263 by PSOM to B cell lymphoma.

4:10 PM Engineering *Shewanella Oneidensis* for Bisphenol a Degradation and Biofilm Formation (ThC2b)

Jiacheng Zhou (Illinois Institute of Technology), *Seok Hoon Hong* (Illinois Institute of Technology)

Bisphenol A (BPA) has been widely used as a plasticizer in the production of synthetic polymers, such as food storage containers and feeding and non-returnable bottles. BPA has drawn global attention due to its ability to interfere with endocrine systems, causing carcinogenicity, immunotoxicity, and embryotoxicity. Wastewater treatment bioprocess barely removes BPA due to the poor BPA degradation ability and efficiency of applicated microorganisms. In this work, we engineered Shewanella oneidensis, commonly used in the biodegradation process of wastewater treatment because of its excellent extracellular electron transfer properties, to enable BPA degradation. We integrated bisdA and bisdB encoding a BPA degradation pathway from Sphingomonas bisphenolicum strain AO1 into S. oneidensis MR1. The engineered S. oneidensis MR1 exhibited over 95% of BPA degradation within 10 min, while the engineered Escherichia coli with the same BPA degradation pathway showed 80%. In addition, we improved the biofilm formation of S. oneidensis by enhancing curli biogenesis and c-di-GMP production. Since biofilms are used to degrade toxic organic compounds during wastewater treatment, we investigate BPA degradation in functional biofilms. This study will reveal the relation between BPA degradation, enhanced electron transfer, and biofilm formation of S. oneidensis.

4:35 PM Mechanical and Structural Characterization of Thin Films (ThC2c)

Mark Haase (Anton Paar) [**canceled**]

Thin films see increasingly wide use, serving as catalysts and catalyst supports, pharmaceutical carriers, protective coatings, and many other applications. Characterization of the structural and mechanical characteristics of these films is critical for their manufacture and their use in the production of other products. In this presentation, we will explore how Atomic Force Microscopy and Gas Sorption can be used to characterize the mechanical and structural properties of both soft and hard coatings, with special attention to nanoscale features.

<u>Poster Session</u>

Thursday, March 18, 2021 (**ThP1**)

5:15 PM Poster Session

Poster 1 **Digitalization of Process Safety – Utilizing Wearables to Conduct Remote Activities Safely (ThP1a)**

Robert Weber (PSRG, Inc.)

The COVID pandemic has shifted the way people work in industrial environments. Process safety activities, like audits, inspections, PSSRs, and other tasks, that were previously conducted by muitidisciplinary teams onsite are now being performed more and more remotely due to social distancing requirements, travel restrictions, reduced operating budgets, and other constraints. However, there is still a need to perform physical observations to meet compliance requirements and maintain safe operations. Digitalization of process safety enables the use of rugged, hard hat mounted, instrinsically safe Android virtual reality technology to record and capture important data which can be communicated real-time to remote Teams, Mentors, Managers/Supervisors, and Customers. This enables planned activities to be performed as scheduled and emergency situations to be observed and diagnosed instantly, so that important decisions may be made immediately rather than deferring critical items. The return on investment (ROI) by deployment of these industrial wearables can be realized after a single use. In this case study which demonstrates the successful deployment of digital, hands-free wearable technology, global leaders in energy, manufacturing and other heavy industries can learn to empower and connect their global workforce while reducing worker errors, improving safety, maintaining compliance, and increasing productivity through digitalization of process safety.

Poster 2 **Techno Economic Analysis of the Modified Mixalco Process (ThP1b)**

Brooke Zidek (Milwaukee School of Engineering),
Chloe Simchick (Milwaukee School of Engineering)

The MixAlco process is a patented biomass conversion technology which relies on the use of fermentation to convert a variety of biomass into useful chemicals. Unlike previous MixAlco designs which model the production of hydrocarbon fuels, this proposed design simulates mixed carboxylic acid production. These have a more competitive selling price than hydrocarbon fuels. For the base case feed rate of 18.5 US tons of biomass per hour, the estimated total capital investment is $28,949,000, and the payback time at a 47.54% ROI is 2.10 years at a minimum selling price range of $1.90-$2.38 per gallon. Sensitivity analysis identified four critical input factors of the process: biomass feed rate, selling price, distribution cost, and biomass composition. Overall, the sensitivity analysis of all four input factors support that the new design is flexible in its ability to support populations of varying sizes as well as different biomass feed rates and compositions.

Poster 3 **Predicting Reaction Mechanism of Electrochemical CO2 Reduction Using Machine Learning (ThP1c)**

Aditya Prajapati (University of Illinois at Chicago)

Understanding the mechanism of an electrochemical reaction could, in principle, be one of the important factors in the accelerated discovery of highly efficient electrocatalysts. Cyclic voltammetry (CV) is one of the techniques providing important mechanistic insight into an electrochemical reaction by the virtue of the change in current density when a reactant or an intermediate species is adsorbed/desorbed on the electrode surface. However, interpreting a CV can be influenced by subjectivity from the experience of the electrochemist. Moreover, quantifiable confidence in such interpretations is wanting. Machine Learning (ML) algorithms can be applied in such cases to circumvent the heuristics in CV interpretations and user subjectivity to present robust, quantifiable confidence in predicting electrochemical reaction mechanisms. One of the most attractive electrochemical reactions in recent years has been the electrochemical CO2 reduction (CO2R) to value-added chemicals due to its potentially high impact on the industries, society, and the environment. This work shows the implementation of an ML model with various classification algorithms(Decision Tree, Random Forest, Back Propagation Neural networks, Probabilistic Neural Networks, and Naïve Bayes Algorithm) to predict the reaction mechanism of CO2R by learning from different data sets of cyclic voltammograms. The simulated and experimental cyclic voltammograms are used to train the neural network to identify the dependence on the parameters like CV scan rates and uncompensated resistance. For each individual CV, the voltammogram serves as an input to the model. The expected output predicts the likelihood of the occurrence of either simple reversible electron transfer reactions or irreversible product formation after an electron transfer reaction. This ML model confirms that the predictions can be made even by simple models as a substitute for the conventional subjective approach.

Poster 4 **Cost Productive Cybersecurity Approach to Securing Plant Operations (ThP1d)**

Pranav Patel (ResiliAnt)

AIChE Midwest Regional Conference

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AIChE Midwest Regional Conference

High School Outreach Program

The American Institute of Chemical Engineers (AIChE) is proud to host Engineering Day for local high school students in concurrent to the AIChE 13th Annual Midwest Regional Conference. This event is a great opportunity for students to explore the exciting profession of a chemical engineer as well as other engineering disciplines. In partnership with Illinois Institute of Technology and University of Illinois at Chicago, this high school outreach program will be hosted virtually with interactive sessions including engineering expos, lab tours, networking with the professionals, and Q&A with the engineering panel! We invite you to discover the world of engineering with us, be inquisitive, and of course, have fun along the way!

Event Schedule

8:30 am **Welcome Session**

8:50 am **Engineering Expo**
Meet current engineering students and check out the projects that they have been working on.

9:50 am **10 Minute Break**

10:00 am **Engineering Lab Tours**
University Engineering Lab Tours, Argonne National Laboratory Tour

11:00 am **30 Minute Lunch Break**

11:30 am **Networking with the Professionals**
Opportunity for small group discussions with engineering professionals and students.

12:30 pm **Keynote Speaker – Dr. Elizabeth Corson**
TomKat Postdoctoral Fellow in Sustainable Energy, Stanford University

1:30 pm **10 Minute Break**

1:40 pm **Engineering Panel**
Learn about the day-to-day activities of practicing engineers and engineering students. Time to ask your most burning questions.

2:40 pm **Closing Remarks**

Dr. Elizabeth Corson is a TomKat Center Postdoctoral Fellow in Sustainable Energy at Stanford University, studying how to recover resources from wastewater through electrochemical nitrate reduction. She completed her Ph.D. in Chemical Engineering at the University of California, Berkeley where she did research on converting carbon dioxide into valuable fuels and chemicals through plasmon-enhanced electrochemical reduction. Originally from Iowa, Elizabeth received her B.S. in Chemical Engineering from the Illinois Institute of Technology in Chicago.

Check out https://hopin.com/events/aiche-engineering-day for more information about the event or email us at aiche.outreach.chicago@gmail.com.

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Calling All Professional Engineers!

"Networking with the Professionals" is a great opportunity for the high school students to learn more about engineering and ask questions in a small interactive group setting. Each group of seven high school students to be paired with one professional engineer and one university engineering student to discuss a career in engineering. Please be prepared to share about your career path and what you love about engineering! If you are interested in participating in the *Networking with the Professionals*, please register for the event using the link below.

https://hopin.com/events/aiche-engineering-day?code=9ucoqp6PKrK6fpeDnIWrtvCni

If you do not have a hopin account, you will need to create one before registering.

MRC 2022

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Chicago - Spring 2022

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