6TH ANNUAL

AIChE® MIDWEST REGIONAL CONFERENCE

March 10-11, 2014

University of Illinois at Chicago

· PROCESS SAFETY · REFINING · BIO-PROCESSING ·

· ENERGY · PROFESSIONAL DEVELOPMENT ·

Presented by the AIChE Chicago Section

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Conference Overview

The AIChE Midwest Regional Conference (MRC) continues into its 6th year. Organized by the **Chicago Local Section** with support from AIChE Technical Programming and hosted by the **University of Illinois, at Chicago**, the MRC provides an opportunity for engineers and scientists in the region to learn about new technologies and network with others in the field. A particular objective of the conference is to build technical relationships between industrial practitioners and researchers in the governmental and academic spheres. Statistics of the technical program include **2 Keynote Lectures**: *Rakesh Agrawal* (Purdue University) and *Hans Fauske* (Fauske & Associates), **28 technical sessions and 99 oral presentations**.

The Monday evening program begins with a **Poster Session**, followed by a buffet dinner and a **Dinner Keynote** Lecture on Food Engineering and the Integrated Bio-refinery by *James Foster* (Director of Process Development Research, Archer Daniels Midland Company).

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

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

On behalf of the conference planning committee we welcome you to the 6th Annual AIChE Midwest Regional Conference and hope you will take advantage of all the opportunities it has to offer.

Jeffery Perl
Conference Chair
Chicago Chem Consultants and University of Illinois at Chicago

Program at a Glance

Monday, March 10, 2014

7:30 AM - 8:30 AM **Continental Breakfast** (Fort Dearborn A)

8:30 AM – 9:30 AM **Morning Keynote** (Illinois B)
Chemical Engineering for a Sustainable Energy Future,
Rakesh Agrawal, Winthrop E. Stone Distinguished Professor, Purdue University

10:00 AM – 11:30 AM **Technical Sessions**
- *Atomic Layer Deposition for Renewable Energy* (Cardinal Room)
- *Biomolecules and Polymers at Interfaces* (White Oak AB)
- *New Problems and Opportunities Facing US Refineries* (Fort Dearborn B)
- *YP Engineering 101* (Illinois A)

11:30 AM – 1:00 PM **Lunch with Middle/High School Outreach Participants**
(Illinois A and Illinois B)

1:00 PM – 2:30 PM **Technical Sessions**
- *Electrical Energy Production and Conversion* (Cardinal Room)
- *Renewables Research and Pilot Operations* (White Oak AB)
- *Energy, Sustainability and the Environment* (Fort Dearborn B)
- *Smart Grid Tutorial* (Illinois A)
- *YP Resume Workshop* (East Terrace)

2:30 PM – 3:00 PM **Networking Break**

3:00 PM – 4:30 PM **Technical Sessions**
- *Advances in Reaction Engineering* (*Cardinal Room*)
- *Biomaterials for Immunological Applications* (*White Oak AB*)
- *Analysis of Financial and Ecological Processes* (*Fort Dearborn B*)
- *YP Engineering without Borders* (*Illinois A*)

4:30 PM – 6:00 PM **Poster Session** (*Illinois C*)

6:00 PM – 7:00 PM **Buffet Dinner** (*Illinois B*)

7:00 PM – 8:00 PM **Dinner Keynote** (Illinois B)
ADM Developments in Food Engineering and the Integrated Biorefinery
James Foster, Director of Process Development Research, Archer Daniels Midland Company

Program at a Glance

Tuesday, March 11, 2014

7:30 AM - 8:30 AM **Continental Breakfast** (Fort Dearborn A)

8:30 AM – 9:30 AM **Morning Keynote** (Illinois B)
An Alternative Methodology Addressing United Nations (UN) Classification Type for Self-Reactive Substances
Hans Fauske, Emeritus President and Regent Advisor, Fauske & Associates

10:00 AM – 11:30 AM **Technical Sessions**
- *Current Thoughts on Process Safety Culture, Near-misses, and Major Incident Prevention* (Cardinal Room)
- *Materials for Biomedical Applications I* (White Oak AB)
- *Advances in Fluidization* (Fort Dearborn B)
- *Undergraduate Chemical Engineering Education, Industrial Needs and Professional Practice Standards* (Illinois A)

11:30 AM – 1:00 PM **Lunch** (Illinois A and Illinois B)

1:00 PM – 2:30 PM **Technical Sessions**
- *Process Safety Quantitative Analysis Developments* (Cardinal Room)
- *Materials for Biomedical Applications II* (White Oak AB)
- *Issues in Emerging Energy Technologies I* (Fort Dearborn B)
- *Engineering for Sustainability* (Illinois A)
- *Corn to Chemicals Industrial Complex I* (Illinois B)
- *YP Mock Interviews* (East Terrace)

2:30 PM – 3:00 PM **Networking Break**

3:00 PM – 4:30 PM **Technical Sessions**
- *Hydraulic Fracturing – Process Overview and Implementation, Water Management, and Impact on Illinois Economy* (Cardinal Room)
- *Engineering Cellular Cardiology* (White Oak AB)
- *Issues in Emerging Energy Technologies II* (Fort Dearborn B)
- *Corn to Chemicals Industrial Complex II* (Illinois B)
- *YP Resolving Conflict in the Workplace* (Illinois A)

6:00 PM – 8:00 PM **Young Professional Networking Social** (Off-Site, see back cover)

Keynote Speakers

8:30 AM Monday, March 10, 2014

Rakesh Agrawal, *Winthrop E. Stone Distinguished Professor of Chemical Engineering at Purdue University*

Title: ***Chemical Engineering for a Sustainable Energy Future***

Abstract: *In the long run, it is likely that all the basic human needs will be met by renewable sources like solar energy. However, there are several challenges associated with harness, storage and use of solar energy to meet our daily needs for food, chemicals, heat, electricity and transportation. In a sustainable future, all these usage must coexist. We will first present some results from our energy systems modeling highlighting the synergistic interactions that exist for transportation sector and production of chemicals. This will be followed by a brief discussion and analysis of candidate processes to produce hydrogen from solar energy and our modeling results for energy storage at giga Watt-hour levels. An exciting aspect of producing fuels and chemicals from biomass is learning to produce the array of molecules that we need with minimum process transformation steps and energy use while maximizing biomass carbon recovery. In this aspect, recent advancements at Purdue by a team of chemists, biologists and chemical engineers will be presented. We will show the new pathways and the associated catalysts that have been developed for the production of fuel and chemicals. On the sun to electricity front, we will present highlights of our research on thin film solar cells via nanocrystal ink based route. We will discuss process and technical solutions leading to power conversion efficiencies that are among the highest for Cu(In,Ga)Se2 and Cu2ZnSnSe4 based solar cells by solution based routes. Finally, if the time permits, we will touch upon the continuing advancements made in the traditional fields such as separations that will still play a vital role in the processes slated for any sustainable energy future.*

Biographical Sketch: *Rakesh Agrawal is the Winthrop E. Stone Distinguished Professor in the School of Chemical Engineering at Purdue University, and previouslya Fellow at Air Products and Chemicals, Inc., until 2004. He was a member of the NRC Board on Energy and Environmental Systems (BEES) and a member of the AIChE's Board of Directors and also its Energy Commission. He has published 116 technical papers and holds 118 U.S. and more than 500 foreign patents. These patents are used in over one hundred chemical plants with total capital expenditure in multibillion dollars. He is a member of the US National Academy of Engineering, a Fellow of the American Academy of Arts and Sciences and a foreign Fellow of the Indian National Academy of Engineering. He is currently on the Technical Advisory boards of five chemical companies. Agrawal received the 2010 National Medal of Technology and Innovation from the U.S. President. Dr. Agrawal received a B. Tech. from the Indian Institute of Technology, in Kanpur, India; a M.Ch.E. from the University of Delaware, and an Sc.D. in chemical engineering from the MIT.*

7:00 PM Monday, March 10, 2014

James Foster, *Director of Process Development Research, Archer Daniels Midland Company*

Title: ***ADM Development in Food Engineering and the Integrated Biorefinery***

Abstract: *The presentation will review some recent projects in food engineering at Archer Daniels Midland Company including increasing fiber in the diet using innovative products such as Fibersol-2® and extruded edible bean powder. There will be a special emphasis on areas chemical engineers have made significant contributions to the products. Additionally there will be a update of the Integrated BioRefinery at ADM. This process breaks down biomass to Cellulose, Hemicellulose and Lignin. These components are converted to Butyl Acrylate and Ethanol.*

Biographical Sketch: James Foster is the Director of Process Development Research for the Archer Daniels Midland Company. In this role he is responsible for industrial process development for the company including the corn milling processes including steeping, ethanol fermentation, bioproducts, biodiesel and industrial chemicals production. Foster has numerous publications and 17 patents to his credit and is on the advisory board for the Iowa State University Center for Crops Utilization Research and completed two terms on the board of the University of Illinois Department of Agricultural and Biological Engineering. Education includes a BS in Chemistry and BS in Mathematics from Loyola University, MS and PhD in Chemical Engineering from the University of Illinois. After working for 15 years in the pulp and paper industry, for the last 15 years he has worked for Archer Daniels Midland.

8:30 AM Monday, March 10, 2014

***Hans K. Fauske**, Emeritus President and Regent Advisor of Fauske & Associates*

*Title: **An Alternative Methodology Addressing United Nations (UN) Classification Type for Self-Reactive Substances***

Abstract: This paper provides an alternative to UN testing (such as A, C, E, F, etc.) using one easy to perform 10 g ARSST test to produce the necessary information (maximum rate of pressure rise) to determine the packaging Classification Type. This approach is consistent with UN Guidelines which allow other procedures to be used provided that adequate correlation has been obtained with the classification tests on a representative range of substances.

Biographical Sketch: Hans K. Fauske is Emeritus President and Regent Advisor of Fauske & Associates, LLC., a wholly owned subsidiary of Westinghouse Electric Company, LLC. Since leaving Argonne National Laboratory in 1980 where he served as the first Director of the Fast Reactor Safety Technology Management Center and was responsible for the planning and management of the DOE program, he has been involved in projects covering a wide range of safety issues. He served as a Senior Consultant to the Industry Degraded Core Rulemaking program (IDCOR) and as a Senior Technical Advisor to the Clinch River Breeder Project. He also provided overall technical direction for the AIChE Design Institute for Emergency Relief Systems (DIERS), which was funded by 28 chemical firms in the U.S.A. and abroad. Currently, he is performing a key role in resolving potential process safety issues and the development of inherently safe nuclear and chemical process reactor concepts. Dr. Fauske has published more than 200 scientific articles and holds numerous patents in the areas of nuclear and chemical process safety. He was a member of the editorial boards of the Journal of Loss Prevention in the Process Industries and the International Journal of Multi-Phase Flow. He has taught at several universities in the U.S.A. and abroad and served as the sixth BASF Renowned Scientist Lecturer from 1989 to 1990. He is a fellow of both the American Nuclear Society and the American Institute of Chemical Engineers. In 1975, he became the first person in the field of reactor technology to receive the University of Chicago Medal for Distinguished Performance at Argonne National Laboratory. In 1982, he became the third recipient of the Tommy Thompson Award, the highest honor that the American Nuclear Society bestows in the field of reactor safety. In 1991, he received the ANS Thermal-Hydraulics Division Technical Achievement Award, in 1992 the prestigious AIChE Donald Q. Kern Award for his significant contributions in the area of nuclear and chemical process safety, and in 1996 the AIChE Robert E. Wilson Award in Nuclear Chemical Engineering for his leadership and contributions in developing methods to help assure safety in the nuclear power and chemical process industries. In 2004, he received the Outstanding Achievement Award, from the University of Minnesota, for demonstrating outstanding achievements in his field on an international level. In 2012, he was awarded the George C. Laurence Pioneering Award for Nuclear Safety by the American Nuclear Society.

Session Presentations
Monday, March 10, 2014

Keynote Session Monday, March 10, 2014 (Illinois B)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
8:30 AM **Opening Remarks**
Gerald W. Wilks, Chair of the AIChE Chicago Local Section (CITGO Petroleum)
8:40 AM **Keynote Introduction**
Sohail Murad (University of Illinois at Chicago)
8:45 AM **Chemical Engineering for a Sustainable Energy Future**
Rakesh Agrawal (Purdue University)

Atomic Layer Deposition for Renewable Energy
Monday, March 10, 2014 (Cardinal Room, **M1A**)
Organizer and Chair: *Yu Lei* (University of Alabama, Huntsville)
10:00 AM **Atomic Layer Deposition for the Synthesis of Nanostructured Catalysts**
Jeffrey W. Elam[1], Christopher Marshall[1], Eric Stach[2], Fabio Ribeiro[2], Jeffrey Greeley[1], Justin Notestein[3], Kenneth Poeppelmeier[1,3], Larry Curtiss[1], Mayfair Kung[3], Peter Stair[1,3], Randy Winans[1], Son Binh Nguyn[3], Junling Lu[1], Yu Lei[1], and Christian Canlas[1] ([1]Argonne National Laboratory, [2]Purdue University, [3]Northwestern University)
10:30 AM **3D TiO2 Nanostructures Grown by High-Temperature ALD for High-Efficiency Photoelectrochemical Anodes**
Xudong Wang (University of Wisconsin-Madison)
11:00 AM **Atomic Layer Deposition on Nanostructured Substrates for Photovoltaics**
Elijah Thimsen (University of Minnesota)

Biomolecules and Polymers at Interfaces
Monday, March 10, 2014 (White Oak AB, **M1B**)
Organizer and Chair: *Shyam V. Vaidya* (Abbott Laboratories)
Co-Chair: *Zachary Schultz* (University of Notre Dame)
10:00 AM **Molecular Organization and Translocation in Nuclear Pore Complexes**
Igal Szleifer, Mario Tagliazucchi (Northwestern University)*, Orit Peleg* (Harvard University)*, Martin Kroger.* (Eidgenössische Technische Hochschule)*, Yitzhak Rabin,* (Bar-Ilan University)
10:20 AM **Thermally Responsive Polymers: New Perspectives on an Old Problem**
Deborah Leckband (University of Illinois at Urbana-Champaign)
10:40 AM **High Throughput SERS Detection Enabled by Fluid Dynamics**
Zachary D. Schultz, Pierre Negri, Kevin T. Jacobs, Matthew Bailey, Oluwatosin O. Dada, and Steven M. Asiala (University of Notre Dame) *and R. Scott Martin* (St. Louis University)
11:00 AM **Differentiation of non-specific binding blockers using Quartz Crystal Microbalance with Dissipation monitoring**
Shyam V. Vaidya, Alfredo R. Narvaez (Abbott Laboratories)

New Problems and Opportunities Facing US Refineries
Monday, March 10, 2014 (Fort Dearborn B, **M1C**)
Organizer and Chair: *Gerald W. Wilks* (CITGO Petroleum)
10:00 AM **Overcoming Shale Oil Processing Challenges**
Ezequiel Vincent, George Duggan (Baker Hughes Incorporated)
10:20 AM **New Crudes and Refinery Corrosion Vulnerability Assessments**
Bernard Schulze (Stress Engineering Services)
10:40 AM **Tower Gamma Scanning – Now a Quantitative Tool**
Lowell Pless (Tracerco)
11:00 AM ***Extending the Life of a High Temperature Refinery Reactor***
Gerald W. Wilks (CITGO Petroleum)*, Jim Edmondson* (Shell Projects & Technology)

YP Engineering 101
Monday, March 10, 2014 (Illinois A, **M1D**)
Organizer and Chair: Julie Gruhn (UOP)
10:00 AM **Relief Valves**
Janet Chu (Sensient)

10:30 AM **How to Use a P&ID**
Eleftherios Avtzis (CB&I)
11:00 AM **Fundamentals of Drying**
Adrian Dee (GEA Barr-Rosin)

Electrical Energy Production and Conversion
Monday, March 10, 2014 (Cardinal Room, **M2A**)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair and Co-Chair: *Satish J. Parulekar and Javier Parrondo* (Illinois Institute of Technology)
1:00 PM **Direct Carbon Fuel Cells - Wetting Behavior of Carbon in Molten Carbonate**
Satish J. Parulekar, Feng Peng, Yue Li, and J. Robert Selman (Illinois Institute of Technology)
1:30 PM **Determination of the Limiting Mechanism of Hole Transfer in Sb2S3/CuSCN Solid-State Solar Cells**
Jeffrey A. Christians, David T. Leighton, and Prashant V. Kamat (University of Notre Dame)
2:00 PM **Cardo-polyetherketone based anion exchange membranes for all-vanadium redox flow batteries**
Sukhwan Yun, Javier Parrondo, and Vijay Ramani (Illinois Institute of Technology)

Renewables Research and Pilot Operations
Monday, March 10, 2014 (White Oak AB, **M2B**)
Organizer and Chair: *April Hoffart* (Archer Daniels Midland Co.)
1:00 PM **Scale-Up Challenges with the Integrated BioRefinery**
Lizz Bendis (Archer Daniels Midland Co.)
1:20 PM **From Process Model to Pilot Plant of the Integrated Biorefinery**
Andrew Chin (Archer Daniels Midland Co.)
1:40 PM **Cellulosic Ethanol: A General Review**
Aarthi Srinivasan (Archer Daniels Midland Co.)
2:00 PM **Improved Process for the Manufacture of Isosorbide**
Naveen Sudharsan (Archer Daniels midland Co.)

Energy, Sustainability and the Environment
Monday, March 10, 2014 (Fort Dearborn B, **M2C**)
Organizer and Chair: *Michael E. Walker* (Northwestern University)
Co-Chair: *Yuan Yao* (Northwestern University)
1:00 PM **Storage, Solar and Wind Electricity: Challenges and Opportunities**
George Crabtree, (University of Illinois at Chicago and Argonne National Laboratory)
1:30 PM **Investigating the Impact of Shale Gas Utilization in Bulk Chemical Production**
Yuan Yao (Northwestern University)
2:00 PM **Grand Challenges Facing the Implementation of Carbon Cap-and-Trade Policy**
Michael E. Walker (Northwestern University)

Smart Grid Tutorial
Monday, March 10, 2014 (Illinois A, **M2D**)
Organizer and Chair: *Donald J. Chmielewski* (Illinois Institute of Technology)
1:00 PM **Smart Grid Tutorial: What? Why? How? and Who?**
Donald J. Chmielewski, Benjamin Omell, David Mendoza-Serrano and Oluwasanmi Adeodu (Illinois Institute of Technology)

YP Resume Workshop
Monday, March 10, 2014 (East Terrace and Monarch, **M2E**)
Organizer: *Julie Gruhn* (UOP)
Chair: *Abigail Jackson* (Tetra Pak)
1:00 PM (Monarch) **The Resume - Making a Good First Impression**
Steve Hair (Peak Technical Staffing)
1:30 (East Terrace, floor 2) **Resume Reviews**
Steve Hair (Peak Technical Staffing)*, Abigail Jackson (Tetra Pak), Jesse Calderon* (BakerRisk)*, Michael Toraason* (BakerRisk)*, Janet Chu* (Sensient), *Julie Gruhn* (UOP)

Advances in Reaction Engineering
Monday, March 10, 2014 (Cardinal Room, **M3A**)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair and Co-Chair: *Dennis O'Brien* (Jacobs) *and Satish J. Parulekar* (Illinois Institute of Technology)
3:00 PM **Catalytic Reactions in Various Configurations of a Two-Reactor System**
Satish J. Parulekar (Illinois Institute of Technology)
3:25 PM **Correlating the Degree of Metal-promoter Interaction to Ethanol Selectivity over MnRh/CNTs CO Hydrogenation Catalysts**
Jingjing Liu[1], Zhao Guo[1], Robert Klie[1], Chris Marshall[2], Jeff Miller[2] and Randall Meyer[1]
([1]University of Illinois at Chicago, [2]Argonne National Laboratory)

3:50 PM **New Insights into Cellulose Pyrolysis Reaction Kinetics**
Heather Mayes, Linda J. Broadbelt (Northwestern University)*, and Gregg T. Beckham* (National Renewable Energy Laboratory)
4:15 PM **On the Development of Portable Atomic Layer Deposition System for Lab Research**
Sathees Kannan Selvaraj, Gregory Jursich, and Christos G Takoudis (University of Illinois at Chicago)

Biomaterials for Immunological Applications
Monday, March 10, 2014 (White Oak AB, **M3B**)
Organizer and Chair: *Michael Gower* (Northwestern University)
3:00 PM **Self-assembled Peptide Immunomodulators**
Joel H. Collier, Rebecca R. Pompano, and Jianjun Chen, Anita S. Chong (University of Chicago)
3:30 PM **Self-Assembled Peptide Amphiphile Micelles as Vaccine Delivery Systems**
Bret D. Ulery[1], Amanda Trent[2], Simon Liang[1], Natalie Simon[1] and Matthew Tirrell[1] ([1]University of Chicago, [2]University of California Santa Barbara)
4:00 PM **Immune Tolerance for Regenerative Medicine**
Lonnie D. Shea, Michael Gower, Woon Teck Yap, Kelan Hlavaty, Samira Azarin, Brian Aguado, Shreyas Rao, Xunrong Luo, Stephen Miller, and Jacqueline Jeruss (Northwestern University)

Analysis of Financial and Ecological Processes
Monday, March 10, 2014 (Fort Dearborn B, **M3C**)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair: *Urmila Diwekar* (VRI-CUSTOM)
3:00 PM **Valuation of Process Stoichiometry in Incomplete Markets**
Fernando Garcia, Jeffery Kantor (University of Notre Dame)
3:30 PM **Controllability of Complex Networks for Sustainable System Dynamics**
Pahola Thathiana Benavides (VRI-CUSTOM and University of Illinois Chicago)*, Urmila Diwekar* (VRI-CUSTOM)*, Heriberto Cabezas* (U.S. EPA)
4:00 PM **Assessing the Benefits of Stochastic Market Clearing**
Naiyuan Chiang and Victor M Zavala (Argonne National Laboratory)

YP Engineers without Borders
Monday, March 10, 2014 (Illinois A, **M3D**)
Organizer: *Julie Gruhn* (UOP)
Chair: *Alan Zagoria* (UOP)
3:00 PM **Engineers without Borders and Your Career**
Alan Zagoria (UOP)**,** *Jessica Chepp* (EWB)

Poster Session
4:30 PM - 6:00 PM Monday, March 10, 2014 (Illinois C)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair and Co-Chair: *Belinda Akpa and Manuela Ayee* (University of Illinois at Chicago)

Dinner Keynote
Monday, March 10, 2014 (Illinois B)
7:00 PM **Keynote Introduction**
Dan Rusinak (Middough)
7:10 PM **ADM Developments in Food Engineering and the Integrated Biorefinery**
James Foster (Archer Daniels Midland Company)

Session Presentations
Tuesday, March 11, 2014

Keynote Session
Tuesday, March 11, 2014 (Illinois B)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
8:30 AM **Volunteer Recognition**
Jeffery P. Perl, Conference Chair (Chicago Chem Consultants)
8:40 AM **Keynote Introduction**
AnnMarie Fauske (Fauske & Associates)
8:45 AM **An Alternative Methodology Addressing United Nations (UN) Classification Type for Self-Reactive Substances**
Hans Fauske (Fauske & Associates)

Current Thoughts on Process Safety Culture, Near-Misses, and Major Incident Prevention
Tuesday, March 11, 2014 (Cardinal Room, **T1A**)
Organizer: *Delmar "Trey" Morrison* (Exponent)
Chair and Co-Chair: *Brenton Cox and Ryan Hart* (Exponent)
10:00 AM **Applying Game Theory to Understand Process Safety Culture**
Sean Dee, Russell Ogle, Delmar "Trey" Morrison (Exponent)
10:30 AM **Using Near Misses to Improve Risk Management Decisions**
Brenton Cox, Sean Dee, Russell Ogle (Exponent)
11:00 AM **Evaluating the Process Safety Culture Implications of Major Incidents: Chemical Release and Explosion at a Plastics Plant**
Andrew Carpenter, Russell Ogle (Exponent)

Materials for Biomedical Applications I
Tuesday, March 11, 2014 (White Oak AB, **T1B**)
Organizer and Chair: *Georgia Papavasiliou* (Illinois Institute of Technology)
Co-Chair: *Eric Brey* (Illinois Institute of Technology)
10:00 AM **Multi-Agent model of Bone Tissue Growth within Porous Biomaterials**
Elif S. Bayrak, Hamidreza Mehdizadeh, Banu Akar, Sami Somo, Eric Brey, Ali Cinar (Illinois Institute of Technology)
10:15 AM **Fibrin Beads for Delivery of Endothelial Colony-Forming Cells**
Jarel K. Gandhi and Eric Brey (Illinois Institute of Technology), *John Fisher* (University of Maryland), *Mervin Yoder* (Indiana University)
10:30 AM **Comparison of different methods for predicting customized drug dosage in superovulation stage of in-vitro fertilization**
Kirti Maheshkumar Yenkie and Urmila Diwekar (University of Illinois at Chicago and VRI-CUSTOM)
10:45 AM **Fibronectin, fibrin, hydrogels and stability – biongineering as a tool for addressing the problems in the chronic wound**
Anand Ramanathan, Raj Desai, Chen Zhang, Zhongyang Wang, Nancy Karuri (Illinois Institute of Technology)
11:00 PM **Immunomodulatory Scaffolds for Enhanced Cell Transplant**
R. Michael Gower, Jesse Zhang, Jeffrey Liu, Christine F. Ricci, Jack G. Graham, Xiaomin Zhang, Lonnie D. Shea (Northwestern University)
11:15 AM **In Vitro testing of Virulence Suppression of P. aeruginosa by phosphate loaded nanoparticles**
Yushu Yin, Fouad Teymour, Georgia Papavasiliou (Illinois Institute of Technology), *Olga Zaborina and John C. Alverdy* (University of Chicago)

Advances in Fluidization
Tuesday, March 11, 2014 (Fort Dearborn B, **T1C**)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology);
Chair and Co-Chair: *Stoyan Nedeltchev* (TU Braunschweig) *and Reza Mostofi* (UOP)
10:00 AM **Comparison of Three Different Entropies in a Fluidized Bed Operated with an Air-Polyethylene System**
Stoyan Nedeltchev (TU Braunschweig)
10:20 AM **CFD Modeling of an FCC Stripper**
Ray Cocco, Allan Issangya, Ted Knowlton, and S.B. Reddy Karri (Particulate Solid Research, Inc)
10:45 AM **Upgrading FCC Performance using Ansys-Fluent**
Reza Mostofi (UOP)

11:10 AM **A New Approach for Prediction of Gas Holdups in a Slurry Bubble Column Operated at Different Conditions**
Stoyan Nedeltchev (TU Braunschweig)

Undergraduate Chemical Engineering Education, Industrial Needs and Professional Practice Standards

Tuesday, March 11, 2014 (Illinois A, **T1D**)
Organizer and Chair: *Jeffery P Perl* (University of Illinois at Chicago and Chicago Chem Consultants)
Co-Chair: *Dennis O'Brien* (Jacobs Consultancy)
10:00 AM **Professional Engineering Licensing Exam Specification – A Model for Chemical Engineering Practice**
Jeffery P. Perl, (University of Illinois at Chicago and Chicago Chem Consultants)
10:30 AM **Teaching and Practicing Modern Chemical Process Control**
Gary Hawkins (Emerson Process Management), *Dennis O'Brien* (Jacobs Consultancy)
11:00 AM **Chemical Engineering at the Rose-Hulman Institute of Technology**
Adam J. Nolte (Rose-Hulman Institute of Technology)

Process Safety Quantitative Analysis Developments

Tuesday, March 11, 2014 (Cardinal Room, **T2A**)
Organizer and Chair: *Peter Herena* (BakerRisk)
Co-Chair: *Charlie Pacella* (BakerRisk)
1:00 PM **Performance-Based Fire & Gas Design**
Murtaza Gandhi (BakerRisk)
1:30 PM **Upcoming changes in IEC 61511, SIS for Process Industries**
Peter Herena (BakerRisk)
2:00 PM **Fundamentals of Quantitative Risk Assessments**
Mike Moosemiller, Mike Toraason, and Jesse Calderon (BakerRisk)

Materials for Biomedical Applications II

Tuesday, March 11, 2014 (White Oak AB, **T2B**)
Organizer and Chair: *Eric Brey* (Illinois Institute of Technology)
Co-Chair: *Georgia Papavasiliou* (Illinois Institute of Technology)
1:00 PM **Polymeric modulation of immune cell function**
Jamie E. Rayahin, Jason S. Buhrman and Richard A. Gemeinhart (University of Illinois at Chicago)
1:15 PM **Electrostatic Unfolding and Interactions of Albumin Driven by pH Changes**
Gali Baler, Marcelo A. Carignano, Guillermo A. Ameer, Igal Szleifer (Northwestern University), *Osvaldo A. Martin, and Jorge A. Vila* (Universidad Nacional de San Luis)
1:30 PM **Development of an Extended Release Drug Delivery System to Treat Choroidal Neovascularization**
Christian R. Osswald,and Jennifer J. Kang-Mieler (Illinois Institute of Technology)
1:45 PM **Hydrogel Stiffness Modulates Adipose Expansion In Vitro**
Marcella Vaicik, Jose Rios, and Eric Brey (Illinois Institute of Technology)
2:00 PM **PEG Hydrogel/Nanoparticle Scaffold Systems for Sustained Delivery of Angiogenic Peptides**
Daniel Young, Georgia Papavasiliou (Illinois Institute of Technology)
2:15 PM **Recombinant melittin protein loaded microspheres for treatment of high grade astrocytoma**
Jason S. Buhrman, Jamie E. Rayahin, and Richard A. Gemeinhart (University of Illinois at Chicago)

Issues in Emerging Energy Technologies I

Tuesday, March 11, 2014 (Fort Dearborn B, **T2C**)
Organizer and Chair: *William Ryan* (University of Illinois at Chicago)
1:00 PM **Biomass Conversion via Thermochemical Conversion to Useful Energy** *Yaroslav Gnatyuk* (University of Illinois at Chicago)
1:30 PM **Carbon Dioxide Storage and Utilization**
Lauren Pankowski (University of Illinois at Chicago)
2:00 PM **Balance of System Technologies Under Development to Lower the Cost of Large PV Plants** *Joshua Barrett* (University of Illinois at Chicago)

Engineering for Sustainability

Tuesday, March 11, 2014 (Illinois A, **T2D**)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair and Co-Chair: *Mustafa Cagdas Ozturk and Emad Ghadirian* (Illinois Institute of Technology)

1:00 PM **CFD Simulation of the Regeneration Process for CO2 Removal using a Regenerable Solid Sorbent**
Emad Ghadirian, S. Zarghami, J. Abbasian and H. Arastoopour (Illinois Institute of Technology)

1:30 PM **Mechanistic Modeling of Fast Pyrolysis of Glucose-based Carbohydrates**
Xiaowei Zhou and Linda J. Broadbelt (Northwestern University)

2:00 PM **Bifurcation Analysis of Wastewater Treatment Operation**
Mustafa Cagdas Ozturk, Arun Kumar Raju Ganesan, Paul R. Anderson, Fouad Teymour (Illinois Institute of Technology)

YP Mock Interviews

Tuesday, March 11, 2014 (East Terrace, **T2E**)
Organizer: *Julie Gruhn* (UOP)
Chair: *Abigail Jackson* (Tetra Pak)

1:00 PM (East Terrace) **Relax - It's just an interview**
Julie Gruhn (UOP)

1:30 (East Terrace) **Mock Interviews**
Julie Gruhn (UOP), *Abigail Jackson* (Tetra Pak), *Jerry Wilks* (CITGO), *Jeremy Isaacs* (Middough), *and Todd MacMillan* (Ecolab)

Corn to Chemicals Industrial Complex I

Tuesday, March 11, 2014 (Illinois B, **T2F**)
Organizer and Chair: *Jeffery P Perl* (University of Illinois at Chicago and Chicago Chem Consultants)

1:00 PM **UIC Senior Process Design - "Corn to Chemicals"**
Jeffery P Perl (University of Illinois at Chicago and Chicago Chem Consultants)

1:05 PM **Corn Germ Utilization: Corn Oil Extraction, Refining, and Biodiesel Production via Supercritical Transesterification**
Jack Blachut, Kunal Gulati, Monika Jonuskeviciute, Paul Schoeneck (University of Illinois at Chicago) *and Dan Rusinak* (Middough)

1:30 PM **Corn Receiving and Steeping Process**
Patrick Coan, Andre Colorina, Alan Reusnow, Jana Rush, Molly Sompolski (University of Illinois at Chicago) *and John Micheli* (Middough)

1:55 PM **Combined Heat and Power for Corn Wet Milling**
Kunal Desai, Roberto Gomez, Mike Kramer, and Paulina Mlynarska (University of Illinois at Chicago) *and Dave Bahr* (Jacobs Consultancy)

2:20 PM **Sorbitol and Dextrose Production from Corn Starch F**
Taras Dykun, Ricardo Plascencia, Patty Rottinghaus, Sarah Wiersema (University of Illinois at Chicago) *and Tom Stephan* (Consultant)

Hydraulic Fracturing – Process Overview and Implementation, Water Management, and Impact on Illinois Economy

Tuesday, March 11, 2014 (Cardinal Room, **T3A**)
Organizer and Chair: *Jordan Ciezobka* (Gas Technology Institute)

3:00 PM **Hydraulic Fracturing – Old Technology in New Places: Process Overview and Technology Evolution**
Jordan Ciezobka (Gas Technology Institute)

3:30 PM **Issues and Challenges in the Management of Flowback Water and Solid Wastes Associated with Shale Gas Development**
Tom Hayes (Gas Technology Institute)

4:00 PM **Hydraulic Fracturing in Illinois - Will it work and what could it mean for Illinois' economy?**
Tom Wolf (Illinois Chamber of Commerce)

Engineering Cellular Cardiology

Tuesday, March 11, 2014 (White Oak AB, **T3B**)
Organizer and Chair: *Katherine Sheehan* (DePaul University)

3:00 PM **Cardiac Tissue Repair by Local Delivery of a Growth Factor from Polymeric Microrods**
Brenda Russell and Golnar Doroudian (University of Illinois at Chicago)

3:25 PM **Rescue of Familial Cardiomyopathies by Modulation of Ca2+ fluxes and Myofilament Response to Ca2+**
Beata M. Wolska (University of Illinois at Chicago)

3:50 PM **p21-activated kinase-1 signaling alters atrial excitation contraction coupling (ecc)**
Katherine Sheehan (DePaul University)*, R. John Solaro, Beata M. Wolska* (University of Illinois at Chicago)

4:15 PM **Synthesis and Characterization of Phosphate-Loaded PEG Diacrylate Hydrogel Nanoparticles by Inverse Miniemulsion Polymerization**
Srivishnu Vadlamudi, Fouad Teymour, Georgia Papavasiliou (Illinois Institute of Technology)

Issues in Emerging Energy Technologies II

Tuesday, March 11, 2014 (Fort Dearborn B, **T3C**)

Organizer and Chair: William Ryan (University of Illinois at Chicago)

3:00 PM **Mitigation Strategies for Beyond Design Basis External Events** *Sandra Parker* (University of Illinois at Chicago)

3:20 PM **Energy Performance Contracting** *Wildivina Rosario* (University of Illinois at Chicago)

3:40 PM **Wave Energy Converter Technology** *Greg Studier* (University of Illinois at Chicago)

4:00 PM **Performance of Hybrid Solar Photovoltaic Thermal Collectors** *Jerad Tintera* (University of Illinois at Chicago)

YP Conflict Resolution Panel

Tuesday, March 11, 2014 (Illinois A, **T3D**)

Organizer and Chair: *Julie Gruhn* (UOP)

3:00 PM **Resolving Conflict in the Workplace** *Taylor Newsom* (BP), *Jerry Wilks* (Citgo), and *Todd MacMillan* (Ecolab)

Corn to Chemicals Industrial Complex II

Tuesday, March 11, 2014 (Illinois B, **T3F**)

Organizer and Chair: *Jeffery P Perl* (University of Illinois at Chicago and Chicago Chem Consultants)

3:00 PM **Corn Wet Milling Germ Separation** *Will Abbott, Justin Barak, Meghan Lapeta, Jong Shin, Sandy Younan* (University of Illinois at Chicago) *and Shannon Brown* (Ambitech)

3:25 PM **Corn Wet Milling Second Grind and Fiber Drying** *Anwar Beker, Leidy Nallely Jimenez, Katarzyna Orbik, Collin Pearsall, Elizabeth Wanic* (University of Illinois at Chicago) *and Jerry Palmer* (Ambitech)

3:50 PM **Reactor Design for Polyols Production** *Ryan Rock, Nathan Liebmann, Andrew McNamara, Elmar Reyes* (University of Illinois at Chicago) *and Bill Keesom* (Jacobs Consultancy)

4:15 PM **Polyols Separation** *Amber May, Steven Priest, Daniel Sobieski, Garrett Youngblood* (University of Illinois at Chicago) *and Dennis O'Brien* (Jacobs Consultancy)

4:40 PM **Water Treatment Facility in Corn Wet Mill Plant** *Mark Hartman, David Hu, Christopher Rebolloso, Ethan Rendlen* (University of Illinois at Chicago) *and Patrick Shannon* (Middough)

5:05 PM **Centrifugal Separation of Starch and Gluten** *Osman Braimah, Mike Nguyen, Ishai Strauss, James Walsh* (University of Illinois at Chicago) *and Jerry Palmer* (Ambitech)

The American Institute of Chemical Engineers
and The University of Illinois at Chicago
WELCOMES MIDDLE SCHOOL STUDENTS
Monday, March 10, 2014

Being an Engineer—Creating A World That Works!

8:30-9:30	STUDENTS ARRIVE AT UIC
9:30-9:35	WELCOME AND OPENING COMMENTS Alma DeLaGarza-Wozniak, Chemical Engineer, UOP
9:35 -9:55	WHAT IS AN ENGINEER? Gerald Smith, Director of Minority Affairs, College of Engineering, UIC
9:55-10:15	STUDENT COMPETITION: WHAT KIND OF ENGINEER AM I? Emceed by Alan Zagoria, UOP Participants: Selected Student Representatives
10:15-10:30	AWESOME CAREERS YOU CAN PURSUE WITH A CHEMICAL ENGINEERING DEGREE Ludwig C. Nitsche, Associate Professor of Chemical Engineering, UIC
10:30 -11:30	THE ENGINEERING EXPERIENCE: A PANEL DISCUSSION Chair: Alan Zagoria, UOP Panelists: Ludwig C. Nitsche, Associate Professor of Chemical Engineering, UIC Young Professional (Abigail Jackson, Tetrapak) 10+ Year Engineer (Alma DeLaGarza-Wozniak, UOP) UIC Students (Monika Jonuskeviciute and Justin Barak)
11:30-12:30	LUNCH & CHAT WITH PROFESSIONAL ENGINEERS A time for personal activity code for travel expenses is conversation with practicing engineers Hosted by UIC and the AIChE Chicago Section
12:30-12:45	HOW TO PREPARE FOR COLLEGE IN MIDDLE SCHOOL Chris Kuypers (COE)
12:45-1:30	PARALLEL ACTIVITIES below Student Groups to rotate Science and Fun with Foams Classroom Shadowing Tour of Senior Design Laboratory (Mechanical and Electrical Engineering) Tour of Illinois Tool Works Laboratory Tour of the Water Resources Laboratory Tour of CAVE

MIDDLE SCHOOL STUDENTS PROGRAM

WELCOME!

This special middle school program is being run in parallel with the American Institute of Chemical Engineers (AIChE) 6th Annual Midwest Regional Conference, whose objective is to build technical relationships between industrial practitioners and governmental and academic researchers. AIChE and UIC's goal is to expose students to the profession of chemical engineering and engineering in general, and give them the opportunity to interact with professional engineers, engineering students, and faculty. We hope you come away from this program with some idea of what chemical engineers do, how they touch your life, and whether you would like to pursue an engineering career. We encourage you to stay engaged, ask questions, and have fun!

SPEAKERS

Gerald A Smith (M.S Marketing)

Gerry is currently the Director of Minority Affairs and the Director of the Minority Engineering Recruitment and Retention Program (MERRP) in the College of Engineering. His responsibilities in Minority Affairs are to manage and engage with organizations across the UIC campus to enhance processes and programs to promote diversity programs. In his role at MERRP, Gerry has advised and mentored undergraduate and graduate students on their academic performance, student success progress and their future career opportunities. Gerry's goal is for his students to successfully complete their course work and achieve their engineering degrees across all of the engineering professions to become innovators and change the world. Gerry has 20 years of experience on the advisory board with the University of Illinois-Chicago MERRP program, along with his 33+ years of IBM Corporation experience where he has managed engineers, consultants and system engineers over his career prior to coming to UIC.

Ludwig Carlos Nitsche (Ph.D.)

Professor Nitsche received bachelor's degrees in Chemical Engineering and Mathematics from the University of Minnesota and a PhD in Chemical Engineering from the Massachusetts Institute of Technology. He also finished a NATO Postdoctoral Fellowship at the University of Cambridge, UK. Ludwig teaches a variety of undergraduate and graduate courses and serves as the Director of Undergraduate Studies in Chemical Engineering. His research focuses on computer modeling of flow and transport processes and biomedical applications in drug delivery and diffusion of drugs/chemical through the skin.

ACKNOWLEDGEMENTS

2014 Conference Organizers

Conference Chair: Professor Jeffrey Perl (UIC)

Middle School Outreach Organizing Committee

Outreach Chair: Alma DeLaGarza-Wozniak (UOP)
Co-Chair: Gerry Smith (UIC)
Co-Chair: Professor Ludwig Nitsche (UIC)
Middle School Outreach Organizing Committee: Alan Zagoria (UOP), Professor Jeff Perl, Professor Don Donald Chmielewski (IIT), Julie Gruhn (UOP), Professor Belinda Akpa (UIC), Rich Isherwood (UOP), Jeff Lullow (UIC)

Presentation Abstracts

Atomic Layer Deposition for Renewable Energy

Monday, March 10, 2014 (Cardinal Room, **M1A**)

Organizer and Chair: *Yu Lei* (University of Alabama, Huntsville)

10:00 AM **Atomic Layer Deposition for the Synthesis of Nanostructured Catalysts** *Jeffrey W. Elam[1], Christopher Marshall[1], Eric Stach[2], Fabio Ribeiro[2], Jeffrey Greeley[1], Justin Notestein[3], Kenneth Poeppelmeier[1,3], Larry Curtiss[1], Mayfair Kung[3], Peter Stair[1,3], Randy Winans[1], Son Binh Nguyn[3], Junling Lu[1], Yu Lei[1], and Christian Canlas[1]* ([1]Argonne National Laboratory, [2]Purdue University, [3]Northwestern University)

The successful transition to an energy economy based on biomass will require radical advances in catalyst science. This challenge demands a new paradigm in catalyst synthesis whereby inorganic components can be assembled at the atomic scale to yield complex, multifunctional catalysts rivaling Nature's enzymes in their specificity. To this end, we have developed a novel approach combining templated synthesis for shape-selectivity with the atomically-precise positioning of discrete functionalities. In this approach we begin with a supporting scaffold for catalyst growth upon which we chemically attach molecular templates. Next, atomic layer deposition is used to build a structure around each template in an atomically precise, layer-by-layer fashion where the thickness and composition can be tuned at each layer. Finally, the template is removed yielding a "nanobowl" defining a structured catalytic environment. The molecular template can be synthesized to contain bulky organic ligands surrounding a catalytic atom or cluster which remains anchored to the bottom of the bowl after ligand removal. Furthermore, one or more layers in the bowl wall can be selected to serve as a co-catalyst (e.g. Lewis acid group) positioned at a well-defined distance from the catalyst at the bottom of the bowl. This presentation will review our recent progress synthesizing, characterizing, modeling, and testing these unique catalytic materials.

10:30 AM **3D TiO2 Nanostructures Grown by High-Temperature ALD for High-Efficiency Photoelectrochemical Anodes** *Xudong Wang* (University of Wisconsin-Madison)

TiO2 possesses a wide range of application potential in hydrogen production, lithium-ion batteries, fuel cells, gas sensors, detoxification, photovoltaic, photocatalysts, and supercapacitors. Its one-dimensional (1D) morphology is expected to exhibiting higher performance in those applications compared to the bulk form. Recently, we demonstrated a novel high-temperature ALD growth of highly uniform single-crystalline TiO2 nanorods over a large area, even inside highly confined submicron-sized spaces. The growth used separated TiCl4 and H2O precursor pulses at 600 degree C. The anisotropic growth of TiO2 crystals is attributed to the combined effects of surface recombination and HCl restructuring at high temperature during elongated purging time. Therefore, the crystal growth is effectively decoupled from precursor vapor concentration, which allows uniform growth of TiO2 NRs inside highly-confined spaces, such as inside anodized aluminum oxide (AAO) channels and among dense Si nanowires. The phase of TiO2 NRs can be tuned from anatase to rutile by raising the deposition temperature. By adjusting the precursor ratio and exposure time, intrinsic defects in TiO2 crystals could be engineered thus narrowing the bandgap of as-synthesized TiO2 NRs and allowing visible light absorption. For the first time, we realized a high-density 3D NW architecture by growing TiO2 NR arrays inside dense and deep Si NW forests. Such 3D structures offered super large surface area as well as excellent charge transport property. Therefore, dramatically enhanced efficiency was obtained when they were used as photoelectrochemical (PEC) anode for water splitting. 3D TiO2 NR arrays opened a new avenue toward high-performance electrodes design for advancing the performance of PEC and photovoltaic devices.

11:00 AM **Atomic Layer Deposition on Nanostructured Substrates for Photovoltaics** *Elijah Thimsen* (University of Minnesota)

Solar energy conversion devices are layered structures comprised of thin films. Atomic layer deposition (ALD) is a layer-by-layer thin film deposition technique that provides angstrom-level thickness control and conformal coverage of the substrate. Since ALD can deposit ultrathin conformal films, it can be used to functionalize the surface of nanostructured materials; wherein the interface plays a significant role in macroscopic performance. If the interfacial behavior is understood, then in certain cases it can be exploited to realize performance that rivals or even surpasses bulk counterparts. An additional benefit is that the ALD mass-deposition rate on nanostructured materials is much higher than flat substrates because of the surface area, which can be 100 to 1000 times higher than the projected area on the substrate. Compared to flat surfaces, the higher mass-deposition rate on nanostructured surfaces makes ALD competitive with other thin film deposition techniques in terms of production rate, which is an essential improvement for ALD to make contributions to many of the components in thin film PV, wherein film thicknesses are often in the range from 0.1 to 10 µm. I will discuss our recent work on the synthesis of various components of thin film PV from a materials perspective.

Biomolecules and Polymers at Interfaces

Monday, March 10, 2014 (White Oak AB, **M1B**)
Organizer and Chair: *Shyam V. Vaidya* (Abbott Laboratories)
Co-Chair: *Zachary Schultz* (University of Notre Dame)

10:00 AM **Molecular Organization and Translocation in Nuclear Pore Complexes** *Igal Szleifer, Mario Tagliazucchi* (Northwestern University)*, Orit Peleg* (Harvard University)*, Martin Kroger.* (Eidgenössische Technische Hochschule)*, Yitzhak Rabin,* (Bar-Ilan University)

In this talk we will describe theoretical predictions for the molecular structure of yeast Nuclear Pore Complex (NPC) and the translocation of model particles. The theoretical approach that we apply is a molecular theory that accounts for the geometry of the pore and the sequence and anchoring position of the unfolded domains of the nucleoporin proteins (the FG-Nups), which control selective transport through the pore. The theory explicitly models the electrostatic, hydrophobic, steric, conformational and acid-base properties of the FG-Nups. The electrostatic potential within the pore, which arises from the specific charge distribution of the FG Nups, is predicted to be negative close to pore walls and positive along pore axis. The positive electrostatic potential facilitates the translocation of negatively charged particles and the free energy barrier for translocation decreases for increasing particle hydrophobicity. The above results agree with the experimental observation that transport receptors which form complexes with hydrophilic/neutral or positively charged proteins to transport them through the NPC, are both hydrophobic and strongly negatively charged. The molecular theory shows that the effects of electrostatic and hydrophobic interactions on the translocating potential are cooperative and non-equivalent due to the interaction-dependent reorganization of the FG-Nups in the presence of the translocating particle. The combination of electrostatic and hydrophobic interactions can give rise to complex translocation potentials displaying a combination of wells and barriers, in contrast to the simple barrier potential observed for a hydrophilic/neutral translocating particle. This work demonstrates the importance of explicitly considering the amino acid sequence and hydrophobic, electrostatic and steric interactions in understanding the translocation through the NPC.

10:20 AM **Thermally Responsive Polymers: New Perspectives on an Old Problem** *Deborah Leckband* (University of Illinois at Urbana-Champaign)

The temperature-dependent solubility of poly(N-isopropyl acrylamide) has been widely exploited to control polymer interactions with proteins and cells. For decades, the common model has been that the thermally triggered collapse and reswelling of poly(N-isopropyl acrylamide) are essential for reversible protein (and cell) adsorption and release from PNIPAM coatings. I will present evidence that contradicts this view, as well as an alternative model for thermally controlled bioadsorption to grafted polymer brushes. Temperature-dependent protein adsorption and cell adhesion behavior are compared with the chain architecture at different temperature, grafting density, and molecular weight. We qualitatively compared these trends with recent theories for protein interactions with brushes in good and poor solvent. These new results suggest alternative design guidelines for tailoring reversible, thermally triggered protein capture and recovery.

10:40 AM **High Throughput SERS Detection Enabled by Fluid Dynamics** *Zachary D. Schultz, Pierre Negri, Kevin T. Jacobs, Matthew Bailey, Oluwatosin O. Dada, and Steven M. Asiala* (University of Notre Dame) *and R. Scott Martin* (St. Louis University)

The plasmonic enhancement of Raman signals provides a sensitive label-free method of chemical analysis. Raman spectroscopy has long provided chemical specific detection; however, the low intrinsic signal requires additional enhancement for trace analyte characterization. This presentation will demonstrate our approach to high sensitivity Raman detection in flow. The Raman enhancements from a planar nanostructure array we developed enable surface enhanced Raman scattering (SERS) measurements on millisecond time scales.1, 2 The combination of these nanostructured surfaces with fluid dynamics enables ultrasensitive, high-throughput Raman characterization. Using hydrodynamic focusing to confine analytes near a planar SERS substrate, we have demonstrated a 1000x better limit of detection over previous reports.3 This detector has successfully been incorporated into capillary electrophoresis separations. We are exploring a microfluidic version of the detector to improve control of fluid dynamics. Our results provide insight into the origins and utility of plasmon enhanced Raman signals for ultrasensitive detection. We believe SERS detection provides a molecularly specific complement for biomedical diagnostics.

(1) Asiala, S. M.; Schultz, Z. D., Characterization of Hotspots in a Highly Enhancing Sers Substrate. Analyst 2011, 136, 4472-4479.
(2) Asiala, S. M.; Schultz, Z. D., Label-Free in Situ Detection of Individual Macromolecular Assemblies by Surface Enhanced Raman Scattering. Chem. Commun. 2013, 49, 4340-4342.
(3) Negri, P.; Jacobs, K. T.; Dada, O. O.; Schultz, Z. D., Ultrasensitive Surface-Enhanced Raman Scattering Flow Detector Using Hydrodynamic Focusing. Anal Chem 2013, 85, 10159-66.

11:00 AM **Differentiation of non-specific binding blockers using Quartz Crystal Microbalance with Dissipation monitoring** *Shyam V. Vaidya, Alfredo R. Narvaez* (Abbott Laboratories)

Excipient proteins play a key role in immuno-reagent storage and processing stability and are fundamental to the assay performance often by reducing non-specific binding (NSB). Immuno-reagent formulations are exposed to varied material surfaces during manufacturing, storage, and their use on automated immuno-analyzers. Understanding interaction of excipient proteins at these surfaces will help with design of better immunoassays. To this effect, interactions at solid-liquid

interfaces were characterized using Quartz Crystal Microbalance with Dissipation monitoring (QCM-D). Adsorption behaviors on surfaces with either hydrophilic (stainless steel and glass) or hydrophobic (polystyrene, polytetrafluoroethylene (PTFE)) properties were studied. Efficiency of excipients towards reducing NSB of plasma proteins from patient samples was compared for BGG, BSA, Mouse IgG, and caseinate. Effect of nonionic surfactants on NSB reduction effectiveness of excipient proteins was also characterized.

New Problems and Opportunities Facing US Refineries

Monday, March 10, 2014 (Fort Dearborn B, **M1C**)
Organizer and Chair: *Gerald W. Wilks* (CITGO Petroleum)

10:00 AM **Overcoming Shale Oil Processing Challenges**
Ezequiel Vincent, George Duggan (Baker Hughes Incorporated)
The amount of shale oil being refined has increased rapidly during the past few years due to their availability and lower price compared to conventional crudes. At first glance these crudes are light, low viscosity, low in sulfur and asphaltenes, and appear to present a high quality crude for refining. Upon closer examination, severe processing issues are likely, and in fact are being reported on a frequent basis. These problems range from storage tank wax deposition, to rapid preheat exchanger and furnace fouling, and increased tower salting. The resultant operational issues have led to cases of reduced throughput and even crude unit shutdowns. This presentation reviews the problems posed by shale oil processing, and presents prediction and control strategies that refiners have used to overcome such challenges.

10:20 AM **New Crudes and Refinery Corrosion Vulnerability Assessments** *Bernard Schulze* (Stress Engineering Services)
Corrosion vulnerability assessments for refinery process units have been performed for a number of years to assist in the development or review of inspection planning activities. These assessments involve the identification of the expected damage mechanisms, based upon the materials of construction and the process environment present. The appropriate inspection techniques are then identified that are most effective in detecting the type of damage expected. The output can include where, when and how often to inspect and ultimately be used for prioritization within a given process unit. This presentation will outline the assessment process and how the introduction of new crudes from shale formations could impact refinery programs.

10:40 AM **Tower Gamma Scanning – Now a Quantitative Tool**
Lowell Pless (Tracerco)
Tower gamma scanning is well established in the process industries as a qualitative tool to help troubleshoot separation towers, both trayed and packed. In this presentation it will be shown that through careful and innovative application of gamma scanning quantitative information about separation towers can be extracted. Examples of trayed towers and packed towers will be presented that illustrate how quantifying gamma scan data can provide more useful information than by traditional qualitative analysis.

11:00 AM ***Extending the Life of a High Temperature Refinery Reactor*** *Gerald W. Wilks* (CITGO Petroleum)*, Jim Edmondson* (Shell Projects & Technology)
The introduction of crudes originating from shale formations and from other tight formations has led to a new series of problems facing US refineries. The new crudes bring with them a variety of chemicals which impact corrosion, fouling, and equipment operations in refineries. NACE recognized this potential problem for refineries, and it formed Task Group 489 titled "Potential Effects of Upstream Additives on Refinery Corrosion and Fouling". This Task Group has already held several meetings, and has developed a database containing over 150 chemicals that might be used in shale and other tight formations to facilitate oil extraction. The task group's goal is to develop guidelines that refineries can use to avoid processing problems with these new crudes. This presentation will provide a summary of Task Group activities, and will solicit input from conference attendees pertaining to this NACE effort.

YP Engineering 101

Monday, March 10, 2014 (Illinois A, **M1D**)
Organizer and Chair: Julie Gruhn (UOP)

10:00 AM **Relief Valves** *Janet Chu* (Sensient)
Provide an understanding of the basic types of pressure relief valves and an introduction on some of the common sizing cases.

10:30 AM **How to Use a P&ID** *Eleftherios Avtzis* (CB&I)
An introduction to piping and instrumentation drawings and how to read P&ID's in conjunction with related drawings.

11:00 AM **Fundamentals of Drying** *Adrian Dee* (GEA Barr-Rosin)
A look at the key technologies involved in drying processes and the selection criteria for choosing the right equipment.

Electrical Energy Production and Conversion

Monday, March 10, 2014 (Cardinal Room, **M2A**)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair and Co-Chair: *Satish J. Parulekar and Javier Parrondo* (Illinois Institute of Technology)

1:00 PM **Direct Carbon Fuel Cells - Wetting Behavior of Carbon in Molten Carbonate** *Satish J. Parulekar, Feng Peng, Yue Li, and J. Robert Selman* (Illinois Institute of Technology)

The Direct Carbon Fuel Cell (DCFC), which uses solid carbon as fuel and molten carbonate as electrolyte, has had resurgence of interest due to very high electrochemical conversion efficiency, nearly 100%, no requirement of fuel reforming, and potential for CO2 capture and sequestration. At the cathode, carbon dioxide is converted into carbonate ions. The main reaction at the anode is generation of carbon dioxide from carbon and carbonate, the net cell reaction being oxidation of carbon to carbon dioxide. Additional reactions that may be occur at the anode are a two-electron reaction resulting in co-generation of carbon dioxide and carbon monoxide and the Boudouard reaction leading to conversion of carbon and carbon dioxide to carbon monoxide, the so-called "carbon corrosion". The performance of DCFC can be appreciably limited by this reaction. The reverse Boudouard reaction has not been studied in solid-melt-gas systems. It is important to study this reaction in conjunction with wetting behavior of carbon in molten carbonate.

With this in mind, the wetting behavior of carbon electrode in molten carbonate, comprised of a Li-K eutectic mixture, was investigated in this study at different temperatures. The wetting behavior is complicated due to reactions occurring at the carbon surface before or after the start of wetting. Before wetting, carbon rods were exposed to a gas atmosphere with varying partial pressures of carbon dioxide to examine the extent of Boudouard reaction and the resulting structural changes in carbon rods. This reaction modifies the lateral surface of carbon electrode due to carbon corrosion, which leads to reduction in interfacial tension between solid carbon and molten carbonate after dipping carbon rods in molten carbonate.

Wetting behavior of carbon rods was studied for a period of 24 hours. The effects of temperature and pre-exposure to varying levels of carbon dioxide on speed of formation of liquid (molten carbonate) meniscus, propagation of liquid film thereafter, and the ultimate length of liquid film were studied. Other characteristics of molten carbonate film also depend on these two variables. During the wetting process, bubble evolution occurred at the surface of carbon electrode not only below the meniscus, but also above the meniscus. This indicates that wetting of carbon electrode in molten carbonate is influenced not only by capillary forces but also by the reverse Boudouard reaction. The reverse Boudouard reaction is promoted at higher temperature, leading to changes to greater extent in the surface structure and therefore solid-liquid and solid-vapor interfacial tensions.

The lateral surfaces of graphite rods before wetting and after wetting, liquid films formed on the graphite rods, and cross-sections of cylindrical carbon rods above and below the meniscus were analyzed using SEM. The liquid films and circular cross-sections of carbon rods were also analyzed using energy-dispersive X-ray spectroscopy (EDX) and distributions and variations in oxygen and potassium were examined. Oxide ions are generated prior to and during wetting of carbon rods and play an important role in surface modification of these prior to and during wetting.

A reaction mechanism based on the experimental observations is proposed. The roles of Boudouard reaction, including its equilibrium characteristics, and oxide ions on surface modification of carbon rods before and after wetting and the implications thereof on wetting behavior of carbon rods are explained satisfactorily by the reaction mechanism.

1:30 PM **Determination of the Limiting Mechanism of Hole Transfer in Sb2S3/CuSCN Solid-State Solar Cells** *Jeffrey A. Christians, David T. Leighton, and Prashant V. Kamat* (University of Notre Dame)

Extremely thin absorber solar cells based on an Sb2S3 absorber have shown promise as inexpensive, solution processable photovoltaics, demonstrating power conversion efficiencies over 6%. In these solar cells, photogenerated electrons and holes are rapidly transferred to TiO2 and a hole conductor, respectively. The mechanism and rate of hole transfer from Sb2S3 to a CuSCN hole conductor is studied using femtosecond transient absorption spectroscopy. As anticipated, the rate of hole transfer from Sb2S3 to CuSCN is dependent on Sb2S3 film thickness, a trend which is attributed to diffusion of trapped holes in the Sb2S3 layer. Modeling of the hole transfer process reveals that the hole transfer is not adequately explained by diffusion limitations alone, and transfer across the Sb2S3-CuSCN interface plays a significant role in limiting the hole transfer rate. For this reason, a model is developed incorporating both diffusion and hole transfer which elucidates the relative contributions of diffusion and interfacial transfer. From this, it is seen that interfacial transfer is the predominate mechanism limiting the rate of hole transfer between Sb2S3 and CuSCN. Finally, the importance of hole transfer in this system is elucidated through photovoltaic measurements on planar Sb2S3/CuSCN solar cells.

2:00 PM **Cardo-polyetherketone based anion exchange membranes for all-vanadium redox flow batteries** *Sukhwan Yun, Javier Parrondo, and Vijay Ramani* (Illinois Institute of Technology)

The all-vanadium redox flow battery (VRFB) is one of the promising energy storage systems which is suitable for large-scale applications. As a separator for the VRFB system, cardo-polyethereketone (PEK-C) based anion exchange membranes (AEM) and organic/inorganic composite AEMs were prepared. N-(Trimethoxysilylpropyl)-N,N,N-trimethylammonium (TMSP-TMA+) was used as the inorganic additive and the PEK-C based AEM was quaternized using trimethylamine. The sulfate ion conductivity of the pristine AEM and the composite AEM with 30wt% TMSP-TMA+ were 3.2 ± 0.4 mS cm-1 and 6.1 ± 0.4 mS cm-1 at 30oC. respectively. Ultimate tensile strength (UST) and elongation at break (EB) of the composite membranes were improved to 27 ± 1 MPa and 48 ± 8 % with 10wt% and 30wt% of TMSP-TMA+, respectively (UST and EB of the pristine AEM were 22.5 ± 2 MPa and 22 ± 4 %, respectively). PEK-C based

AEMs were stable during VRFB operation (at 30 mAcm-2) for 50 charge/discharge cycles and showed coulombic and energy efficiencies of 98% and 80%, respectively.

Renewables Research and Pilot Operations

Monday, March 10, 2014 (White Oak AB, **M2B**)
Organizer and Chair: *April Hoffart* (Archer Daniels Midland Co.)

1:00 PM **Scale-Up Challenges with the Integrated BioRefinery** *Lizz Bendis* (Archer Daniels Midland Co.)

Archer Daniels Midland, Company, in partnership with the Department of Energy, is currently piloting an Integrated BioRefinery (IBR) for commercial evaluation. The goal of this project is to cost effectively convert corn stover into usable products. Corn stover is the residue left on the field after corn is harvested and includes stalks, husks, and cobs. By successfully achieving this goal, the process will take what has traditionally been a waste material and make value-added products including ethanol, butyl acrylate, and lignin.

There are many complications with this process that have been discovered through the work of developing a pilot plant. This presentation will focus on the development of the current pilot plant and the future challenges that can be solved to make the IBR an economically viable operation.

1:20 PM **From Process Model to Pilot Plant of the Integrated Biorefinery** *Andrew Chin* (Archer Daniels Midland Co.)

The process for the Integrated BioRefinery is designed to convert corn stover into value added products, such as acrylates and ethanol. A new pilot plant has been designed and built to demonstrate this process.

In order to properly design and size equipment for the pilot plant, an ASPEN Plus model was created to determine the process flows, pressures, and other design specifications. During construction, ongoing process changes and equipment limitations caused the actual process specifications to deviate from the model. This presentation will focus on what some of these changes were and how these challenges were reconciled in ASPEN Plus.

1:40 PM **Cellulosic Ethanol: A General Review** *Aarthi Srinivasan* (Archer Daniels Midland Co.)

Archer Daniels Midland Co. (ADM) has been the leading producer of the biofuels, such as ethanol and biodiesel, which are alternative fuels that are currently available to consumers. Lignocellulosic biomass represents a potential source of carbohydrates for fermentation into fuels and chemicals. Feedstock supply and environmental impacts are not seen as significant barriers to the widespread use of ethanol from cellulosic biomass. Although conversion economics is a key obstacle to overcome, a cost competitive process appears to be a possible solution in the near future.

2:00 PM **Improved Process for the Manufacture of Isosorbide** *Naveen Sudharsan* (Archer Daniels midland Co.)

Isosorbide is a heterocyclic compound that is derived from glucose. It is a white solid that is prepared from the catalyzed dehydration of sorbitol. Crude isosorbide could be used in bisphenol A (BPA) replacement, as a monomer for polyurethanes or as a feedstock for surfactants. Refined Isosorbide is used as a monomer for polyesters, polyurethanes, polycarbonates, as a humectant in paints and as a chemical feedstock for epoxy resins, solvents, plasticizers, surfactants. The current process is developed to achieve a cost-effective, scalable process for the manufacture of highly pure, color-free isosorbide with an enhanced shelf life. The process improvements are a fine-tuned synthesis utilizing design of experiments methodology, deployment of membrane ultrafiltration, simulated moving bed ion-exclusion, strong acid cation and strong base anion resins for ion-exchange, an activated carbon polish and wiped-film molecular still purification with concurrent antioxidant co-distillation. This process optimization improves final yield, while increasing purity to >99.5% and reducing color from >200 on the APHA scale to nearly non-detectable. Preliminary cost models predict that the addition of unit operations will produce a superior product at a commercially viable price.

Energy, Sustainability and the Environment

Monday, March 10, 2014 (Fort Dearborn B, **M2C**)
Organizer and Chair: *Michael E. Walker* (Northwestern University)
Co-Chair: *Yuan Yao* (Northwestern University)

1:00 PM **Storage, Solar and Wind Electricity: Challenges and Opportunities** *George Crabtree,* (University of Illinois at Chicago and Argonne National Laboratory)

Transportation and the electricity grid are on the cusp of transformative change driven by the advent of all-electric cars and widespread deployment of wind and solar electricity. The bottleneck for both transformations is high performance, inexpensive storage of electricity. The Joint Center for Energy Storage Research (JCESR) introduces a new paradigm for battery research and development integrating discovery science, battery design, research prototyping and manufacturing collaboration in a single highly interactive organization. JCESR's mission is to develop next-generation batteries with five times the energy density and one fifth the cost of today's commercial batteries within five years. The challenges of achieving these transformative goals and their impact on renewable solar and wind electricity will be discussed.

1:30 PM **Investigating the Impact of Shale Gas Utilization in Bulk Chemical Production** *Yuan Yao* (Northwestern University)

The recent rise in U.S. shale gas production has broad implications to next-generation manufacturing in the chemicals industry. This presentation discusses a model for bulk chemicals production from shale gas in the United States and

explores the potential energy-use and GHG emissions implications of possible large-scale feedstock and technology shifts for producing bulk chemicals over the next several decades. Such analyses are important for assessing shale gas's role in meeting long-term U.S. energy use and emissions reductions targets, as well as for identifying specific technological pathways that can be encouraged by policy and incentives in a proactive fashion. This presentation will discuss the evaluation of alternative technologies for producing high-value bulk chemicals in a framework that captures the material and energy flows, processes, and life-cycle impacts of these alternative technologies, as well as the capital and infrastructure systems necessary to support them.

2:00 PM **Grand Challenges Facing the Implementation of Carbon Cap-and-Trade Policy** *Michael E. Walker* (Northwestern University)

Reducing greenhouse gas (GHG) emissions from industrial sources is one of the most complex challenges facing engineers today. Cap-and-trade policies are a useful and proven market-based strategy that can influence and incentivize emissions reductions from industrial sources. However, there are a number of 'Grand Challenges' facing the implementation and effectiveness of such policies. This presentation highlights the numerous challenges that can arise and strategies to overcome them, based on work performed with the California Air Resources Board and the California cap-and-trade program. This presentation will cover the following issues: multiple product outputs, carbon leakage, system boundaries, carbon credit allocation, influence of raw material and product quality, technology variations between covered facilities, data availability, and the ability of industries to adapt to emissions reduction constraints.

Smart Grid Tutorial

Monday, March 10, 2014 (Illinois A, **M2D**)
Organizer and Chair: *Donald J. Chmielewski* (Illinois Institute of Technology)

1:00 PM **Smart Grid Tutorial: What? Why? How? and Who?** *Donald J. Chmielewski, Benjamin Omell, David Mendoza-Serrano and Oluwasanmi Adeodu (Illinois Institute of Technology)*

This tutorial presentation will attempt to answer the titled questions: What are the smart grid opportunities for the chemical process industry? Why do these opportunities exist? How should a plant be operated to exploit these opportunities? Who will benefit from smart grid coordination? Specifically, the notion of real-time electricity prices will be introduced and shown to be the result of power industry deregulation coupled with the expected increase in renewable power generation. Then, a number of examples will be presented to illustrate how real-time prices can be exploited. These will expose the software and hardware requirements as well as revenue increase expectations. Finally, the question of investment costs versus revenue gains will be discussed, and methods for assessing the net present value of a proposed smart grid project will be presented.

YP Resume Workshop

Monday, March 10, 2014 (East Terrace and Monarch, **M2E**)
Organizer: Julie Gruhn (UOP)
Chair: Abigail Jackson (Tetra Pak)

1:00 PM (Monarch) **The Resume - Making a Good First Impression**
Steve Hair (Peak Technical Staffing)

A resume is your introduction to your future employer. Come hear how to make a good first impression and bring a copy of your resume for a one on one review. The resume review team represents a diverse group of chemical engineering industries and are available to help you make sure your resume looks its best when you hand it off to possible employers.

1:30 (East Terrace, floor 2) **Resume Reviews**
Steve Hair (Peak Technical Staffing)*, Abigail Jackson (Tetra Pak), Jesse Calderon* (BakerRisk)*, Michael Toraason* (BakerRisk)*, Janet Chu* (Sensient), *Julie Gruhn* (UOP)

Advances in Reaction Engineering

Monday, March 10, 2014 (Cardinal Room, **M3A**)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair and Co-Chair: *Dennis O'Brien* (Jacobs) *and Satish J. Parulekar* (Illinois Institute of Technology)

3:00 PM **Catalytic Reactions in Various Configurations of a Two-Reactor System** *Satish J. Parulekar* (Illinois Institute of Technology)

A comprehensive analysis of static and dynamic behavior of catalytic reactions occurring in two coupled CSTRs is presented. The examples considered pertain to a catalytic reaction exhibiting inhibition by reactant and an enzyme-catalyzed reaction subject to substrate inhibition. A single well-mixed reactor may operate at up to three steady states. The configurations considered are divided into two classes - (C1) reactors with identical feed composition and space time and (C2) reactors with different feed composition and different space times.

The reactors in configuration class C1 need not have identical volumes and volumetric feed, effluent, and exchange rates. Each reactor has feed and effluent streams and therefore can operate independently of the other. The reactors may have one-way interaction (reactors in series) or two-way interaction. A two-reactor system may admit up to nine steady states at least at very low interaction rates. Three of these steady states, symmetric steady states, correspond to identical composition in the two reactors. The remaining steady states, the asymmetric steady states, correspond to different composition in the two reactors and are admissible over a range of

interaction rates. The six asymmetric steady states exhibit multiple pairing sets with two or more limit points. Numerical illustrations reveal the rich steady state structure of the reaction scheme in coupled reactors and wide variety of dynamics of the two-reactor system. The steady states are tracked systematically as the interaction rate is varied. The steady state pairings are altered with change in feed composition and space time. These alterations are associated with emergence of up to four additional steady states. Three types of interaction are considered: (1) equal two-way, (2) unequal two-way, and (3) one-way.

Much more interesting steady state and dynamics patterns are observed in configurations belonging to class C2. Some of the reactor configurations considered here include (1) reactors with different feed composition and space time, (2) reactors in series with one-way interaction, (3) reactors in series with two-way interaction to account for backmixing or recycle, and (4) reactors with dead zones. Interesting patterns of emergence and disappearance of steady states are observed as the extent of interaction between the two reactors in the two-reactor system is varied. A two-reactor system may admit up to nine steady states. Unlike the symmetric steady states in class C1 which remain fixed as interaction between the two reactors is varied, in class C2, all steady states vary in terms of composition in each reactor as the interaction is varied.

The catalytic reaction exhibiting inhibition kinetics does not lead to periodic states in two-reactor systems. The two-reactor system is operationally more flexible and more robust vis-a-vis single reactor. Emergence of additional steady states reveals that the two-reactor system is an example of a complex system.

3:25 PM **Correlating the Degree of Metal-promoter Interaction to Ethanol Selectivity over MnRh/CNTs CO Hydrogenation Catalysts** *Jingjing Liu[1], Zhao Guo[1], Robert Klie[1], Chris Marshall[2], Jeff Miller[2] and Randall Meyer[1]* ([1]University of Illinois at Chicago, [2]Argonne National Laboratory)

Multi-walled carbon nanotubes (MCNTs) were used in this work as a support for Rh based catalysts for high pressure (20 bar) CO hydrogenation. The starting 3wt% Rh/CNTs catalysts were loaded with 1wt% and 2wt% Mn promoter, respectively, in order to study the effect of metal-promoter interactions for ethanol synthesis. Both STEM and EXAFS results showed ~1 nm Rh particles in promoted as well as the unpromoted catalysts, STEM and EELS results verified the enhanced metal-promoter interaction when the amount of Mn promoter increased from 1wt% to 2wt%. The enhancement in the degree of metal-promoter interaction leads to an increase in the ethanol selectivity. Moreover, due to the nature of CNTs (low Z number), the Mn-Rh interactions could be observed at atomic resolution during the STEM-EELS characterization, and the promoter phase is confirmed as Mn(II) oxide by XANES and EELS.

3:50 PM **New Insights into Cellulose Pyrolysis Reaction Kinetics** *Heather Mayes, Linda J. Broadbelt* (Northwestern University)*, and Gregg T. Beckham* (National Renewable Energy Laboratory)

Biomass fast pyrolysis is a promising technology for the thermal conversion of biomass to liquid fuels. With less-severe operating temperatures than gasification, fast pyrolysis produces a primarily liquid product, which requires less-costly equipment for processing and storage than a vapor product. Currently, improvements to make this technology more economically attractive are hampered by a lack of understanding of the reaction chemistry. Computational molecular science offers tools to examine fleeting transition states, knowledge of which can aid in rational catalyst and process design. This talk will share our recent efforts in revealing cellulose pyrolysis reactions using density functional theory. We will discuss how we revealed a new mechanism which overturned conventional wisdom the formation of the main product, as well as how a promising platform chemical is produced.

4:15 PM **On the Development of Portable Atomic Layer Deposition System for Lab Research** *Sathees Kannan Selvaraj, Gregory Jursich, and Christos G Takoudis* (University of Illinois at Chicago)

Increasing popularity of atomic layer deposition process in the areas beyond conventional semiconductor industry attracts considerable interest in the development of lab-scale atomic layer deposition system for research purpose. This presentation will discuss the design and development of a portable atomic layer deposition system built to study the properties of ultra-thin films for energy, semiconductor and biomaterial applications. Successful industrial implementation of the ALD process along with scale-up aspects will also be discussed in the presentation.

Biomaterials for Immunological Applications

Monday, March 10, 2014 (White Oak AB, **M3B**)

Organizer and Chair: *Michael Gower* (Northwestern University)

3:00 PM **Self-assembled Peptide Immunomodulators** *Joel H. Collier, Rebecca R. Pompano, Jianjun Chen, and Anita S. Chong* (University of Chicago)

The self-assembly of engineered peptides and proteins has become a prominent strategy for creating biomaterials. Advantages of these systems include precise compositional definition, control over topology and nanostructure, and the ability to combine multiple different functional components in a modular way. Peptide and protein assemblies are also capable of strongly engaging the immune system, but relatively few design rules exist for exploiting this immunogenicity (for example to create chemically defined vaccines) or for avoiding it (for example in tissue repair or cell delivery). In this talk, the type of immune responses raised by these materials will be

described, in particular their ability to raise strong antibody responses without significant inflammation. In addition, their modularity enables the specific combination of precise ratios of B cell and T cell eptiope peptides, which profoundly influences not only the strength but also the phenotype of the immune response.

3:30 PM **Self-Assembled Peptide Amphiphile Micelles as Vaccine Delivery Systems** *Bret D. Ulery[1], Amanda Trent[2], Simon Liang[1], Natalie Simon[1] and Matthew Tirrell[1]* ([1]University of Chicago, [2]University of California Santa Barbara)

Whole-killed and live-attenuated vaccines have been tremendously effective in preventing pathogenic infections, but can be associated with undesirable side effects. Subunit vaccines that deliver just the peptide antigen of interest have been shown capable of stimulating an immune response, but are generally weak immunogens on their own requiring strong adjuvants (non-specific immunostimulants) to be effective. In order to enhance the immunogenicity of peptide vaccines, new delivery systems must be designed. Peptide amphiphiles are unique biomaterials consisting of a hydrophilic peptide conjugated to a hydrophobic moiety that self-assemble in water into micelles comprised of a hydrophobic tail core and hydrophilic peptide corona. These micelles allow for the presentation of hundreds to tens of thousands of peptides on the surface of each micelle. Peptide amphiphile micelles also crowd peptides within their coronas providing an artificial tertiary structure which induces desirable peptide secondary structure. Since peptides vaccines are often delivered in low local concentrations lacking proper secondary conformation, peptide amphiphile micelles provide a novel platform to improve host immune responses to peptide vaccines. This presentation will detail our recent research utilizing peptide amphiphile micelles for immunological applications.

4:00 PM **Immune Tolerance for Regenerative Medicine** *Lonnie D. Shea, Michael Gower, Woon Teck Yap, Kelan Hlavaty, Samira Azarin, Brian Aguado, Shreyas Rao, Xunrong Luo, Stephen Miller, and Jacqueline Jeruss* (Northwestern University)

A central component for many tissue engineering approaches is a biomaterial scaffold, which provides a tool to modulate the local environment with the objective of promoting development or regeneration into a function tissue. The response of the immune system to the injury or implanted scaffold is critical, as an inflammatory response can further exacerbate the initial injury and the survival and function of endogenous or exogenous progenitor cells. We have employed biomaterials as a platform to modulate the immune response locally and systemically. Biomaterial scaffolds have been modified with the localized delivery of cytokines and chemokines as a means to modulate the immune cell populations within and around the scaffold. Local immunomodulation has been employed enhancing survival of transplanted cells and to protect the transplanted cells from attack by the immune system. We have also employed this approach to attract metastatic cells as a component within a system for the early detection of cancer. Furthermore, we have developed nanoparticles modified with antigens that can be delivered systemically as a means to tolerize the host against these antigens. Particles modified with allogeneic antigens have enabled long-term survival and function of allogeneically transplanted cells in the absence of immunosuppression.

Analysis of Financial and Ecological Processes

Monday, March 10, 2014 (Fort Dearborn B, **M3C**)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair: *Urmila Diwekar* (VRI-CUSTOM)

3:00 PM **Valuation of Process Stoichiometry in Incomplete Markets** *Fernando Garcia, Jeffery Kantor* (University of Notre Dame)

A key aspect in the design and optimization of chemical processes is their economic feasibility. This paper utilizes basic notions in process modeling and quantitative finance to propose a valuation strategy for commodity chemical operations. The primary objective is to gain a deeper understanding of the underlying reactions, stoichiometry, mass and energy balances of a complex chemical process by imposing a minimal set of assumptions regarding the uncertain nature of price dynamics in the commodity markets. Employing a framework developed by Shinnar (Shinnar 1981, Shinnar 1988}, Hildebrandt and Glasser (Hildebrandt 2009, Patel 2005, Patel 2007) for chemical stoichiometry and thermodynamics we establish a modern stochastic interpretation of 'economic potential' as proposed by Douglas (Douglas 1988).

A process model is formulated using the 'simple process' concept of (Hildebrandt 2009, Patel 2005, Patel2007a})that combines basic chemical stoichiometry and thermodynamics for process targeting. We demonstrate the construction investment portfolios comprised of commodities and a risk-free asset that bound the payoff of a simple process model. The value of investment portfolio establishes bounds on the 'fair' price for leasing a unit of capacity of this chemical process. Because the underlying assets cannot span the dynamics of this portfolio the market is 'incomplete', which results in the existence of a range of prices. A linear programming problem is solved to obtain the upper and lower bounds to the prices of this process lease, or what in quantitative finance is known as the bid-ask price (Cerny 2010). Tighter bounds are established by introducing second order stochastic dominance -- the natural generalization of conditional value at risk -- to measure preferences of risk-averse operators.

Incomplete markets subject participants to some degree of financial risk. A key point of this study will be to determine efficient ways to hedge this risk and minimize the likelihood of incurring a deficit.

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[7] Aleš Černý. Mathematical Techniques in Finance: Tools for Incomplete Markets . Princeton University Press, 2nd edition, 2010.

3:30 PM **Controllability of Complex Networks for Sustainable System Dynamics** *Pahola Thathiana Benavides* (VRI-CUSTOM and University of Illinois Chicago)*, Urmila Diwekar* (VRI-CUSTOM)*, Heriberto Cabezas* (U.S. EPA)

Successful implementation of sustainability ideas in ecosystem management requires a basic understanding of the often non-linear and non-intuitive relationships among different dimensions of sustainability, particularly the system-wide implications of human actions. This basic understanding further includes a sense of the time scale of possible future events and the limits of what is and is not likely to be possible. With this understanding, systematic approaches based on control theory can then be used to develop policy guidelines for the system. Therefore, controllability of the system is very important to determining long term sustainability of the system. A recent article in the journal Nature (1) presents a new analytical approach to study the controllability of complex systems. We apply this approach to three dynamic systems developed to study the sustainability of our planet. These three systems consist of an ecosystem based on wild and domesticated compartments, the ecosystem model with an industrial system and a simple economic model, and an integrated model involving the ecosystem, industrial systems, and energy producers. We argue that controllability of this system is linked with the long term sustainability, and we present our arguments in the light of previous studies of these systems.

(1) Liu, Y. Y., Slotine, J. J., Barabási, A. Controllability of complex networks. Nature. 2011, 473, 167

4:00 PM **Assessing the Benefits of Stochastic Market Clearing** *Naiyuan Chiang and Victor M Zavala* (Argonne National Laboratory)

We present a new stochastic programming formulation for day-ahead markets. We show that the formulation provides consistent pricing and enables a more transparent participation of suppliers and consumers with uncertain capacities. We also discuss how stochastic clearing can benefit large consumers with flexible demands and storage capabilities.

YP Engineers without Borders

Monday, March 10, 2014 (Illinois A, **M3D**)
Organizer: *Julie Gruhn* (UOP)
Chair: *Alan Zagoria* (UOP)

3:00 PM **Engineers without Borders and Your Career** *Alan Zagoria* (UOP)**,** *Jessica Chepp* (EWB)

Engineers without Borders is a volunteer organization where engineers (and non-engineers) of all skills, experience levels and backgrounds can make a real difference in the quality of life of the communities we partner with. Whether you are travelling or working at home, EWB offers not only a challenging and rewarding way to apply your technical and people skills, but also provides the opportunity to gain experience and skills that will make you a better engineer.

Poster Session

4:30 PM - 6:00 PM Monday, March 10, 2014 (Illinois C)
Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)
Chair and Co-Chair: *Belinda Akpa and Manuela Ayee* (University of Illinois at Chicago)

Poster abstracts will be distributed on-site.

Current Thoughts on Process Safety Culture, Near-Misses, and Major Incident Prevention

Tuesday, March 11, 2014 (Cardinal Room, **T1A**)
Organizer: *Delmar "Trey" Morrison* (Exponent)
Chair and Co-Chair: *Brenton Cox and Ryan Hart* (Exponent)

10:00 AM **Applying Game Theory to Understand Process Safety Culture** *Sean Dee, Russell Ogle, Delmar "Trey" Morrison* (Exponent)

Deficiencies in conduct of operations and operational discipline (COO/OD) can lead to a decline in the quality of an organization's process safety culture and an increase in the likelihood of process safety incidents. This presentation first introduces some basic concepts from game theory and applies them to the methodology of assessing an organization's process safety culture. We will describe a conceptual framework for the implementation of the process safety assessment process with balanced positive and corrective actions. Assessment guidelines typically focus on the negative outcomes - identifying and correcting gas and deficiencies. This paper argues that the assessment process must also use the positive outcomes - the compliance successes - to provide positive reinforcement to the process safety culture.

Implementing this strategy is consistent with pragmatic management practices and is supported by empirical studies in behavioral science. Finally, this paper discusses how these ideas fit within the framework of AIChE/CCPS and API guidance documents. Both AIChE/CCPS and API offer recent guidance documents on how to conduct effective assessments of process safety management systems.

10:30 AM **Using Near Misses to Improve Risk Management Decisions** *Brenton Cox, Sean Dee, Russell Ogle* (Exponent)

In the process safety literature it is often claimed that the analysis of near-miss incidents can improve process safety performance. However, empirical research has demonstrated that near-miss events are often interpreted by staff as marginally successful outcomes of the process safety management system, leading to riskier behavior due to lower perceived risk. In other words, experiencing a near-miss incident can result in the false conclusion that the original risk was over-estimated. To be effective, the analysis of near-misses must be grounded in an objective evaluation of the event, the outcome, and the severity of the alternative outcomes' consequences.

In this presentation, several examples are given where a near-miss incident preceded a serious incident with significant human injury or property damage. If the near-miss had been investigated, properly evaluated, and appropriate corrective actions been implemented, the more severe incident would likely not have occurred. A recurring theme in these examples is the underestimation of consequence severity, i.e., the misinterpretation of the near-miss as a high-probability, low-consequence severity scenario rather than a narrowly averted low-probability, high-consequence severity scenario. A deliberate consideration of the lower probability, more severe consequence scenario may have facilitated a more thoughtful evaluation of corrective actions.

We will discuss a methodology for evaluating near-misses. It combines events and causal factors charting with barrier analysis to identify the safeguards involved in the near-miss. The near-miss event is then evaluated across the range of potential consequences, and the significance of each identified safeguard is considered. In cases where the severity of the consequence had been underestimated, corrective actions consistent with corporate risk management guidelines should be considered. An equally important outcome of this analysis is the effective communication of the risk at operational and managerial levels of the organization.

11:00 AM **Evaluating the Process Safety Culture Implications of Major Incidents: Chemical Release and Explosion at a Plastics Plant** *Andrew Carpenter, Russell Ogle* (Exponent)

An uncontrolled release of vinyl chloride monomer occurred in a processing building at a plastics manufacturing facility. The release was ignited leading to a catastrophic vapor cloud explosion that killed five workers, severely injured three more, and caused extensive damage throughout the facility. The U.S. Chemical Safety and Hazard Investigation Board (CSB) determined that this incident occurred when an operator drained a pressurized PVC reactor instead of a depressurized reactor that was in the process of being cleaned. The Chemical Safety Board concluded that the cause of the incident was Human Error.

One of our significant findings was that workers at the facility routinely defeated a safety interlock while cleaning the reactors. By defeating this interlock, an operator could open a drain isolation valve more quickly than designed. Facility management had identified and attempted to eliminate this unsafe practice prior to the incident. However, while prior incidents and near misses had alerted management to the possibility of a release, the potential severity of consequences was not understood or embraced by management or the workforce. We will provide some suggestions for using case studies to emphasize elements of process safety.

Materials for Biomedical Applications I

Tuesday, March 11, 2014 (White Oak AB, **T1B**)

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

Co-Chair Name: *Eric Brey* (Illinois Institute of Technology)

10:00 AM **Multi-Agent model of Bone Tissue Growth within Porous Biomaterials** *Elif S. Bayrak, Hamidreza Mehdizadeh, Banu Akar, Sami Somo, Eric Brey, Ali Cinar* (Illinois Institute of Technology)

Repair of bone tissue defects above the critical size using tissue engineering biomaterials modified with signaling molecules and cells with osteogenic potential has become the center of attention considering the limitations and drawbacks of autografting and allografting techniques. The number of variables that contribute to the formation of engineered tissues and the multi-cellular response to these signals present a challenging optimization problem that must be addressed for the success of bone tissue formation. A computational model that can realistically simulate the behavior of such systems over time would be beneficial for many different theoretical and practical purposes. Agent-based modeling (ABM) is a powerful technique for modeling of multi-cellular biomedical systems where cells can be represented as autonomous, interacting agents. In this study, a multi-layer ABM is presented to simulate bone tissue growth and vascular network formation within porous biodegradable growth factor releasing scaffolds. Scaffold vascularization is essential for cells to survive and form functional tissue. In our multi-layer model, one layer describes the events occurring within the scaffold and diffusion of soluble factors, the second layer describes angiogenesis, focusing on the individual behavior of endothelial cells for forming the blood vessel network, and the third layer simulates the behavior of stem cells differentiating and regenerating the bone tissue. This computational framework is used to investigate cellular response to structural changes of

biomaterials and optimize the growth factor release from the scaffolds.

10:15 AM **Fibrin Beads for Delivery of Endothelial Colony-Forming Cells** *Jarel K. Gandhi and Eric Brey* (Illinois Institute of Technology), *John Fisher* (University of Maryland), *Mervin Yoder* (Indiana University)

Delivery of endothelial cells has potential as a therapeutic treatment for ischemic tissues. One potential source of endothelial cells for therapeutic applications is endothelial colony-forming cells (ECFCs), which can be obtained from umbilical cord or adult peripheral blood. Although the most common method of endothelial cell delivery has depended on saline-suspended bolus injection, delivery in a biomaterial scaffold may improve survival and function. Fibrin, a natural polymer, has shown promise as a biomaterial for support of endothelial cell growth and tube-like structure assembly. We describe a robust method for developing fibrin microbeads for ECFC delivery. Fibrin microbeads are formed using sodium alginate as a structural template, and the size, swelling and structural properties of the microbeads were controlled by the needle gauge and composition and concentration of the pre-gel solution. ECFCs were suspended in the fibrin beads and had a cell viability of 54% ± 4% post gelation compared to 85% ± 6% for human umbilical vein endothelial cells. By implementation of dynamic culture using a perfusion bioreactor, ECFCs viability is maintained long term over static culture. ECFC delivery can be optimized by dynamic culture using fibrin microbeads.

10:30 AM **Comparison of different methods for predicting customized drug dosage in superovulation stage of in-vitro fertilization** *Kirti Maheshkumar Yenkie and Urmila Diwekar* (University of Illinois at Chicago and VRI-CUSTOM)

In vitro fertilization (IVF) is one of the highly pursued assisted reproductive technologies worldwide. The IVF procedure is divided into four stages: Superovulation, Egg-retrieval, Insemination/Fertilization and Embryo transfer. Superovulation is the most crucial stage in IVF, since it involves external injection of hormones to stimulate development and maturation of multiple oocytes. The maximum amount of effort and money goes into superovulation. Although numerous advancements have been made in IVF procedures, little attention has been given to modifying the standard protocols based on a predictive model. Currently, the same protocol is followed for every patient. In reality every patient responds differently and hence the proposition to modify the amounts of drug administered based on the patient's initial treatment response is a reasonable approach. The modification of drug dose if based on a well developed mathematical model which takes into account the variability in the follicle growth dynamics as well as the desired outcome thus increasing the predictive value of the method. A model for the follicle growth dynamics and number as a function of the injected hormones and patient characteristics has been developed and validated. Based on this model, the dosage of the hormones to stimulate multiple ovulation or follicle growth is predicted by using the theory of optimal control. The objective of successful superovulation is to obtain maximum number of mature oocytes/follicles within a particular size range. Using the model and optimal control theory the optimal dose and frequency of medication customized for each patient is predicted.

The optimal control problem is solved by different methods like the maximum principle and discretized non-linear programming. The problem is solved with and without constraints to check the variation in the dosage amounts and size of follicles at the retrieval time. The results from different approaches are compared.

10:45 AM **Fibronectin, fibrin, hydrogels and stability – biongineering as a tool for addressing the problems in the chronic wound** *Anand Ramanathan, Raj Desai, Chen Zhang, Zhongyang Wang, Nancy Karuri* (Illinois Institute of Technology)

In a significant proportion of the population in the United States, a small break in the skin can lead to loss of limb or life due to of impaired wound healing. In hard to heal or chronic wounds, fibronectin, an integral part of the cellular scaffold or extracellular matrix in the wound bed is degraded. Chronic wounds do not heal because cells involved in tissue repair, need specific cues in fibronectin to attach, migrate, proliferate and assemble a tissue extracellular matrix.

Our laboratory envisions the chronic skin wound as presenting two main problems: (i) Fibronectin degradation and (ii) the lack of an extracellular matrix on which the tissue can be rebuilt. Our research addresses these two main problems by two main thrusts:

(a) Developing polymer conjugates of fibronectin that are biologically active and proteolytically stable

(b) Synthesizing biologically functional extracellular matrix mimics that are based on composites of hydrogels and fibronectin functional domains.

We present a library of conjugates of polymer and fibronectin that can be used to screen for stable and bioactive conjugates. It also demonstrates how polymeric materials conjugated to fibronectin domains can be used to stimulate extracellular matrix assembly in fibroblasts.

11:00 PM **Immunomodulatory Scaffolds for Enhanced Cell Transplant** *R. Michael Gower, Jesse Zhang, Jeffrey Liu, Christine F. Ricci, Jack G. Graham, Xiaomin Zhang, Lonnie D. Shea* (Northwestern University)

Biomaterial scaffolds are central to many regenerative strategies as they create a space for tissue growth and provide support for cell adhesion and migration. Porous scaffolds have been developed for islet transplant and are able to reverse diabetes with a fraction of the islets that can be isolated from a mouse pancreas. However, transplant of allogeneic and xenogeneic tissue, which is of clinical relevance, requires administration of immunosuppressive drugs, which increases patient susceptibility to infection and cancer. In this talk, I will

describe approaches to control inflammation and the immune response following islet transplant on scaffolds without immunosuppressives. Co-transplant of regulatory T cells protects islet transplants from autoimmune rejection and promotes systemic tolerance to islet antigens, effectively curing autoimmune diabetes. While scaffold-based delivery of immunomodulatory factors decreases inflammatory cell infiltration, modulates cytokine expression, increases regulatory T cell infiltration and Foxp3 expression, and significantly extends islet graft survival in mice. As biological components of allogeneic or xenogeneic origin, such as stem cells, are incorporated into regenerative approaches, modulation of the immune response will be necessary to prevent tissue rejection. Controlling the local immune environment, such as directing the differentiation, activation, or trafficking of immune cells, may be a promising alternative to systemic immunosuppression for the protection of transplanted tissue.

11:15 AM **In Vitro testing of Virulence Suppression of P. aeruginosa by phosphate loaded nanoparticles** *Yushu Yin, Fouad Teymour, Georgia Papavasiliou* (Illinois Institute of Technology)*, Olga Zaborina and John C. Alverdy* (University of Chicago)

Patients exposed to extreme physiological stress as a result of surgical interventions are prone to lethal gut-derived sepsis. Previous studies have shown that under these conditions local phosphate concentrations become depleted in the intestinal tract contributing to a bacterial signaling mechanism that promotes the transition to virulence of the lethal bacterial pathogen P. aeruginosa. To address this issue we have developed an inverse mini-emulsion process for producing phosphate-loaded nanoparticles (NPs) capable of releasing phosphate over a time period of several days. Two nanoparticle (NP) variants have been prepared, one involving phosphate (NP-Pi), the other hexa-metaphosphate, or polyphosphate (NP-PPi). We have also prepared a control consisting of phosphate-free NPs by repeated washing of NPs produced by the same process. All variants were tested for virulence suppression of P. aeruginosa in vitro. In vitro assays were used to detect virulence expression by P. aeruginosa under low phosphate conditions with suspended NPs. To ensure appropriate control groups, washed nanoparticles (NP) served as one control and two dissolved salt samples (phosphate, Pi, and polyphosphate, PPi) were used as additional control. In all experiments a blank control, with only a fixed concentration of bacteria in the media was utilized. By examining the normalized virulence signal the order of signal in media with the same concentration of Pi from high to low is: NP-Pi, Pi, NP-PPi, and PPi. The results indicate that the NP-PPi sample is the most effective for suppressing virulence. It should also be noted that we tested the bacteriostatic effect of all samples and incorporated this in the comparison of normalized signals. The NPs display a strong bacteriostatic effect which is currently being explored.

Advances in Fluidization

Tuesday, March 11, 2014 (Fort Dearborn B, **T1C**)

Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology);

Chair and Co-Chair: *Stoyan Nedeltchev* (TU Braunschweig) *and Reza Mostofi* (UOP)

10:00 AM **Comparison of Three Different Entropies in a Fluidized Bed Operated with an Air-Polyethylene System** *Stoyan Nedeltchev* (TU Braunschweig)

A new type of entropy was defined and extracted from photon count time series measured by gamma-ray densitometry facility in a fluidized bed (0.438 m in ID) operated with an air-polyethylene (mean particle size: 675 µm) system. The fluidized bed was equipped with a porous plate distributor (15-40 µm). The new entropy was compared with the Kolmogorov entropy (KE) and maximum information entropy (IEmax) values reported earlier by Nedeltchev et al. (2012). The aim of the comparison was to determine which of these entropies is most suitable for flow regime identification, i.e. which entropy is most sensitive to the flow regime changes. Nedeltchev et al. (2012) found that both KE and IEmax exhibit a well-pronounced minimum which identifies the minimum fluidization velocity Umf. In the range of the examined superficial gas velocities, no other transition velocity was identified. In the bubbling fluidization regime both parameters decreased monotonously. The new type of entropy can identify not only the Umf value but also the upper boundary of the transition flow regime (so-called minimum bubbling velocity) and the onset of the turbulent fluidization regime. This is its main advantage in comparison to the other two entropies. The results from several scintillation detectors (recording the photon counts) positioned strategically around the fluidized bed are presented.

*Nedeltchev, S., F. Ahmed and M. Al-Dahhan, "A New Method for Flow Regime Identification in a Fluidized Bed Based On Gamma-Ray Densitometry and Information Entropy", Journal of Chemical Engineering of Japan 45, 197-205 (2012)

10:20 AM **CFD Modeling of an FCC Stripper** *Ray Cocco, Allan Issangya, Ted Knowlton, and S.B. Reddy Karri* (Particulate Solid Research, Inc)

Strippers are commonly used in fluidized catalytic cracking (FCC) and fluid coking unit operations for the removal of valuable hydrocarbon products from the circulating catalyst. Failure to remove these vapors from the catalyst results in a loss of valuable products and will result in excessively high temperatures from the regenerator. Thus, entrained and adsorbed hydrocarbon vapors in these unit operations are typically removed from the catalyst in fluidized bed strippers using steam. One of the most common types of strippers is the disk and donut tray stripper. Alternating trays of annular rings and conical hats are used to enhance the mass transfer between the solids and stripping gas by (i) breaking up and slowing down the bubbles or voids, (ii) dividing the stripper into several axial stages for more plug flow behavior, and (iii)

limiting gas mal-distribution due to gas-bypassing [Issangya, et al., 2006, 2008].

However, disk and donut strippers are not without their problems. Although these types of strippers can achieve high stripper efficiencies, their effectiveness is limited to flooding. In many cases, this flooding limits the productivity of the entire fluidized catalytic cracking or coker units. Adding vent holes to the disk and donut stripper can minimize this problem without sacrificing stripper efficiencies [Revault, et al.]. Disk and donut strippers with these vent holes can operate at approximately 20% higher solids fluxes than disk and donut strippers without these holes.

In order to better understand the hydrodynamic differences in disk and donut strippers with and without vent holes, computational fluid dynamic (CFD) models using CPFD-Software's Barracuda® were used to study the differences in the gas and solid hydrodynamics for disk and donut strippers with and without vent holes.

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Rivault, P., Nguyen, C., Laguerie, C., Bernard, J. R., Aquitaine, E., Counter Current Stripping Dense Circulating Beds eEffect of the Baffles, in Fluidization VIII, Large, J.-F., Laguerie, C., eds., Engineering Foundation, New York, pp 725 - 732, 1995,

Snider, D., "An incompressible Three-Dimensional Multiphase Particle-in-Cell Model for Dense Particle Flows," Journal of Computational Physics, vol. 170, no. 2, pp. 523–549, 2001.

10:45 AM **Upgrading FCC Performance using Ansys-Fluent**
Reza Mostofi (UOP)

Using computational methods, some examples are shown to demonstrate the use of CFD (computational fluid dynamics) to improve FCC (fluid catalytic cracking) performance in industrial units. CFD is being used widely in chemical industry to help in design, improve or troubleshoot different units. FCC units are an important part of a refinery and it involves multiphase flows where not all the required physics are known. In this presentation three examples will be discussed.

11:10 AM **A New Approach for Prediction of Gas Holdups in a Slurry Bubble Column Operated at Different Conditions**
Stoyan Nedeltchev (TU Braunschweig)

The experimental gas holdups in a slurry bubble column (0.095 m in ID) were predicted successfully by using the classical theoretical expression for the gas-liquid interfacial area and an empirical correlation for the interfacial area (referred to slurry volume) estimation (Schumpe et al., 1987). In such a way, the gas holdup was related to superficial gas velocity and effective (or apparent) viscosity. Both correlations were initially assumed to be equal and then the obtained gas holdups were corrected due to the fact that the classical definition of the interfacial area is strictly valid for rigid spherical bubbles. Under the examined conditions the bubbles have oblate ellipsoidal shape (Tadaki numbers in between 2 and 6 or in some cases up to 12.5) and that is why a correction is needed. It was found that the correction factor is a single function of the Eötvös number. The Sauter-mean bubble diameter was calculated from the correlation of Lemoine et al. (2008).

Air was used as a gas phase and the following gas-liquid systems were studied: tetralin-alumina (Al2O3) (particle size dp=10.5×10-6 m), ligroin-polyvinylchloride (dp=82×10-6 m), ligroin-polyethylene (A and B) (dp=24 and 106×10-6 m), water-activated carbon (dp=5.4×10-6 m), sodium sulfate (Na2SO4)-alumina (dp=10.5×10-6 m) and Na2SO4-kieselguhr (dp=6.6×10-6 m). The gas holdups were measured visually (from the change of the dispersion height) under ambient conditions. The unaerated height of the suspension was kept constant (at 0.85 m). Two different single tubes (Ø 3×10-3 m and Ø 0.9×10-3 m) were used as gas distributors. The difference between each predicted and experimental gas holdup was always within ± 20 %.

Undergraduate Chemical Engineering Education, Industrial Needs and Professional Practice Standards

Tuesday, March 11, 2014 (Illinois A, **T1D**)

Organizer and Chair: *Jeffery P Perl* (University of Illinois at Chicago and Chicago Chem Consultants)

Co-Chair: *Dennis O'Brien* (Jacobs Consultancy)

10:00 AM **Professional Engineering Licensing Exam Specification – A Model for Chemical Engineering Practice**
Jeffery P. Perl, (University of Illinois at Chicago and Chicago Chem Consultants)

The National Council for the Examination of Engineers and Surveyors (NCEES) oversees professional engineering licensure in the United States. The author has served on the Chemical Engineering PE Exam Committee along with 25-30 practicing ChE and faculty for the past 6 years as well as an adjunct professor at UIC where he teaches the capstone engineering design course. This paper will examine the juxtaposition of academic instruction and PE licensure requirements.

10:30 AM **Teaching and Practicing Modern Chemical Process Control** *Gary Hawkins* (Emerson Process Management), *Dennis O'Brien* (Jacobs Consultancy)

Industrial chemical manufacturing is focused on the selection and tuning of process controllers, sensors and distributed control systems. Modern academic instruction relies heavily upon the use of Laplace Transform based modeling for process control, with little to no end use application. This session will explore the class-room/control-room interface and how it might be improved with a little "feedback" from both camps.

11:00 AM **Chemical Engineering at the Rose-Hulman Institute of Technology** *Adam J. Nolte* (Rose-Hulman Institute of Technology)

I will present an overview of the chemical engineering program at the Rose-Hulman Institute of Technology, including our approaches to undergraduate education, meeting accreditation criteria, and assuring our graduates are well-prepared to meet current industrial needs.

Process Safety Quantitative Analysis Developments

Tuesday, March 11, 2014 (Cardinal Room, **T2A**)
Organizer and Chair: *Peter Herena* (BakerRisk)
Co-Chair: *Charlie Pacella* (BakerRisk)

1:00 PM **Performance-Based Fire & Gas Design** *Murtaza Gandhi* (BakerRisk)

From the increasing interaction between Safety Instrumented Systems (SIS) and Fire & Gas Systems(FGS) has arisen the argument that FGS should be treated as SIS, and therefore under the purview of the SIS Design standard ISA 84.

Some operating companies have had difficulty when attempting to apply simple techniques (such as Layers of Protection Analysis) to FGS that are commonly applied to traditional SIS. This is because FGS is a mitigative system rather than a preventive system like traditional process SIS.

The ISA 84 committee released a technical report (TR7) in 2010 that provides guidance on the evaluation of FGS effectiveness. The presentation will review the basic principles of the FGS lifecycle, and discuss methods operating companies or consultants can apply to determine FGS performance requirements that are practical to achieve, more reliable and consistent with good safety.

1:30 PM **Upcoming changes in IEC 61511, SIS for Process Industries** *Peter Herena* (BakerRisk)

The International Society of Automation (ISA) and International Electrotechnical Commission (IEC) have been developing standards and guidance documents for industry for several decades. These standards range in concept from electrical design requirements to the evaluation of Safety Instrumented System (SIS) performance, among many other topics. ISA and IEC published an essentially identical standard, Functional Safety for Safety Instrumented Systems for the Process Industry Sector, with the exception of a “grandfather clause” in the ISA 84 version. Both of these standards include the concept that SIS should be designed, installed, operated and maintained as part of a holistic safety lifecycle.

Although at present the standards are highly aligned, the management teams for the two standards bodies are different; the IEC 61511 board is considering major changes in quantitative performance analysis for SIS performance for their 2014-2015 update, which are under debate within the ISA 84 technical committee leadership. This presentation will review some of the potential changes, and what the impact of those changes may be to SIS analysis practitioners, SIS integrators, and end-users.

2:00 PM **Fundamentals of Quantitative Risk Assessments** *Mike Moosemiller, Mike Toraason, Jesse Calderon* (BakerRisk)

Quantitative Risk Assessments, commonly referred to as QRAs, estimate the cumulative process risk posed by operation of a facility. QRAs are widely used in the petrochemical industry, and the scope may include onsite and/or offsite personnel (less commonly, the results of a QRA can be expressed in purely economic or environmental terms). To calculate risk the analysis starts by calculating all potential outcomes in the event of an accident or failure, typically using dispersion models. The outcomes can be used to determine vulnerabilities to onsite and offsite occupants of the facility in question. These vulnerabilities can then be combined with the frequency of each outcome to determine risks. The frequencies are typically developed using initiating event failure rate data coupled with conditional probabilities such as wind direction, probability of ignition, etc.

QRAs hold a significant advantage over purely consequence-based Facility Siting Study, or FSS. QRAs allow facilities to pinpoint high risk locations, versus just high consequence locations. Very high consequence facilities may pose minimal risk to onsite or offsite personnel due to high levels of built-in reliability, and therefore may require less or no mitigation than a purely consequence-based assessment would have suggested. Where mitigation is warranted, consequence-based studies are useful primarily in identifying opportunities for improvement with respect to event prevention and structural upgrades. Risk evaluations offer the additional benefits of managing hazards through initiating event frequency reduction (e.g. improved inspections), altering the conditional modifiers (e.g. better ignition source controls) or managing the exposure (e.g. personnel relocations). Risk-based evaluations are also more amenable to cost-benefit analyses.

This presentation will review the fundamentals of a quantitative risk assessment. This will include the development of the consequence-based model and the incorporation of those calculations into a risk based model. The presentation will also discuss situations where consequence models may apply more appropriately than typical quantitative risk assessments.

Materials for Biomedical Applications II

Tuesday, March 11, 2014 (White Oak AB, **T2B**)
Organizer and Chair: *Eric Brey* (Illinois Institute of Technology)
Co-Chair: *Georgia Papavasiliou* (Illinois Institute of Technology)

1:00 PM **Polymeric modulation of immune cell function** *Jamie E. Rayahin, Jason S. Buhrman and Richard A. Gemeinhart* (University of Illinois at Chicago)

Hyaluronic acid is a ubiquitous polymer found in the extracellular matrix of humans and many animals. Favorable chemical and mechanical properties of the polymer have made

it a popular choice for the development of controlled drug delivery systems as well as implant coatings for bioengineered products. Despite its widespread use, many have reported differing physiologic activities of the polymer based on its size, which has led to confusion in the literature. In the context of bioengineered systems, immune response is of vital importance. The macrophage phenotype has been shown to be a powerful predictor of response to stimulus. We have shown that hyaluronic acid has differential effects on macrophage polarization, dependent on its molecular weight. Elucidation of these effects not only supports and defines their utility in a bioengineering approach, but also allows us to explore polymers in the context of disease development and progression, regulation and plasticity of macrophage function, and development of favorable synthetic analogues.

1:15 PM **Electrostatic Unfolding and Interactions of Albumin Driven by pH Changes** *Gali Baler, Marcelo A. Carignano, Guillermo A. Ameer, Igal Szleifer* (Northwestern University)*, Osvaldo A. Martin, and Jorge A. Vila* (Universidad Nacional de San Luis)

A better understanding of protein aggregation is bound to translate into critical advances in several areas, including the treatment of misfolded protein disorders and the development of self-assembling biomaterials for novel commercial applications. Because of its ubiquity and clinical potential, albumin is one of the best-characterized models in protein aggregation research; but its properties in different conditions are not completely understood. We carried out all-atom molecular dynamics simulations of albumin to understand how electrostatics can affect the conformation of a single albumin molecule just prior to self-assembly which we have observed experimentally. We then analyzed the tertiary structure and solvent accessible surface area of albumin after electrostatically triggered partial denaturation. The data obtained from these single protein simulations allowed us to investigate the effect of electrostatic interactions between two proteins. The results of these simulations suggested that hydrophobic attractions and counter ion binding may be strong enough to effectively overcome the electrostatic repulsions between the highly charged monomers. This work contributes to our general understanding of protein aggregation mechanisms, the importance of explicit consideration of free ions in protein solutions, provides critical new insights about the equilibrium conformation of albumin in its partially denatured state at low pH, and may spur significant progress in our efforts to develop biocompatible protein hydrogels driven by electrostatic partial denaturation.

1:30 PM **Development of an Extended Release Drug Delivery System to Treat Choroidal Neovascularization** *Christian R. Osswald,and Jennifer J. Kang-Mieler* (Illinois Institute of Technology)

Choroidal neovascularization (CNV) secondary to age-related macular degeneration has become the most common cause of vision loss in elderly patients in the US. Several FDA-approved drug therapies for CNV require monthly bolus intravitreal injections of antiangiogenic agents. Less frequent administration via controlled and extended release of these agents is needed to improve upon current therapies and lessen the potential side-effects of intravitreal injections. To address these issues, we have developed a drug delivery system consisting of poly(lactic-co-glycolic) acid (PLGA 75:25) microspheres suspended within a thermoresponsive, injectable poly(N-isopropylacrylamide)-based hydrogel. Radiolabeled ovalbumin (44.3 kDa) was used as a model protein for ranibizumab (Mw 48.4 kDa), an FDA-approved anti-VEGF therapeutic for CNV. The microspheres had an average diameter of 7.7μm±5μm and encapsulation efficiency of 21.8%±3.9%. Release profiles were conducted at 37°C under mild agitation. The initial burst (IB, <24 hr) was 20.2%±0.01% followed by t1/2 release kinetics. Ovalbumin was released beyond 12 weeks with a second burst release beginning after 9 weeks. When suspended within the hydrogel, the IB significantly dropped to 5.6%±0.59% ($p=1.6\times10^{-5}$), likely due to the hydrogel providing some degree of resistance to the IB. However, subsequent release was not significantly affected. As ovalbumin is of similar molecular weight to ranibizumab, it is expected that these results will translate well to future controlled release studies of ranibizumab using our drug delivery system.

1:45 PM **Hydrogel Stiffness Modulates Adipose Expansion In Vitro** *Marcella Vaicik, Jose Rios, and Eric Brey* (Illinois Institute of Technology)

Animal studies can provide insight into the role of the extracellular matrix (ECM) in adipose function, but do not allow for precise control over environmental conditions. Historically, two-dimensional (2D) substrates have been used to investigate cell–ECM interactions. However, cells in vivo are in a 3D environment surrounded by ECM. The functional response of cells to ECM is different when cells are confined to a monolayer in a 2D versus a 3D culture system. In this study, we used poly(ethylene glycol) diacrylate (PEGDA) hydrogels to study adipose expansion in 3D culture. We are interested in the influence of ECM properties on the expansion, differentiation, and function of adipose tissue. This study has shown that utilizing PEGDA hydrogels it is possible to restrict the expansion and influence the function of adipocytes by modulating the stiffness of the hydrogels.

2:00 PM **PEG Hydrogel/Nanoparticle Scaffold Systems for Sustained Delivery of Angiogenic Peptides** *Daniel Young, Georgia Papavasiliou* (Illinois Institute of Technology)

Rapid and stable neovascularization of implantable scaffolds remains an ongoing challenge in tissue engineering and regenerative medicine. Neovascularization is highly dependent on the interaction of cells with key signals of the native extracellular matrix (ECM). Synthetic hydrogels of PEG diacrylate offer controllable environments for investigating the

role of matrix properties and ECM signaling molecules on neovascularization. While most studies have incorporated the use of growth factors in scaffolds to stimulate scaffold neovascularization, the role of angiogenic peptide molecules on this process is not entirely clear. We are investigating the feasibility of sustained release of angiogenic peptides within proteolytically degradable hydrogel scaffolds in promoting neovascularization. This is achieved through the use of angiogenic loaded PEG hydrogel nanoparticles that allow for sustained release of the peptide. Nanoparticle crosslink density is modified to vary the release kinetics of the peptides. Current efforts are focused on the use of fluorescently tagged peptides to more precisely quantify release kinetics from nanoparticles. Preliminary studies indicate sustained release of peptides from PEG nanoparticles up to 12 days. Physical entrapment of proangiogenic peptides in hydrogel scaffolds demonstrates significantly higher vascular in vitro after two weeks. Future studies will examine the bioactivity of proangiogenic peptides released from the nanoparticles and their effect on 3D vascular invasion in hydrogel scaffolds.

2:15 PM **Recombinant melittin protein loaded microspheres for treatment of high grade astrocytoma** *Jason S. Buhrman, Jamie E. Rayahin, and Richard A. Gemeinhart* (University of Illinois at Chicago)

With a median survival of 15 months, grade IV astrocytoma, or glioblastoma, is among the most feared diagnosis in medicine, and its prognosis has remained largely unchanged. Melittin is a cell lytic peptide derived from the venom of the Apis cerana honeybee and has shown promise in glioblastoma treatment. Protein therapeutics are widely active in the body and are prone to aggregation and degradation: both processes leading to inactivation of the molecule. Hydrogels have shown promise in protecting proteins from extracellular hazards, but modes of reversible protein attachment to hydrogels are lacking. We developed a novel protein anchor based on natural affinity of the glutathione s-transferase (GST) to its cofactor glutathione (GSH). We have shown that GSH fused to the green fluorescent protein (GFP), or melittin, can be readily attached to poly(ethylene glycol) diacrylate (PEGDA) hydrogels. We have engineered a thrombin cleavage site between the GST and the fused therapeutic protein as a proteolytic releasing factor, and have shown physiologic levels of thrombin can release either GFP or melittin in a relatively short time frame (< 1 hour). GST-melittin induces significantly lower cell death in U118 MG than GST-melittin with physiologic levels of active thrombin. Finally, we show that thrombin mediated melittin release from a small (subtherapeutic) number of PEGDA microspheres can induce morphologic changes in U118 MG cancer cells that occurs prior to cell death. Due to the ease of creation, and the already high numbers of therapeutic proteins being purified with GST fusion anchors, we believe the GST/GSH anchor to be a promising component of future protein delivery systems.

Issues in Emerging Energy Technologies I

Tuesday, March 11, 2014 (Fort Dearborn B, **T2C**)

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

1:00 PM **Biomass Conversion via Thermochemical Conversion to Useful Energy** *Yaroslav Gnatyuk* (University of Illinois at Chicago)

Biomass can be converted into useful energy such as steam, heat, electricity, oil and even into transportation fuel by thermochemical conversion technology. There are vast stores of biomass domestically available in the U.S. and thus it can create a positive, sizeable impact in the future of renewable fuels. According to a report from "Biomass as feedstock for Bioenergy and Bioproducts Industry" nearly 1300 million dry tons of biomass resource potential can be used for fuel and electricity in America alone. This is enough to produce 2/5 of electricity for the whole nation or enough to replace 1/3 of annual gasoline use by 2030. However, this is not an easy process to accomplish.

This paper will explore the proper fuel sources for biomass, different technology processes (specifically fluidized bed) that achieve the conversion of biomass to useful energy; the different type of products and byproducts manufactured and distributed to consumers. In addition, this paper will examine the challenges of operating existing thermochemical processes today. And finally, this paper will provide a future financial and political outlook for the emerging thermochemical process technology and demand for energy in the U.S.

1:30 PM **Carbon Dioxide Storage and Utilization** *Lauren Pankowski* (University of Illinois at Chicago)

The purpose of this paper is to explore the various processes and technologies that exist or are under development today to permanently store or utilize carbon dioxide captured from a large point source, such as a fossil-fueled power plant. The focus of this paper will not be on how to capture and purify the carbon dioxide, but rather on what can be done with it after it has been captured. There are two broad categories of carbon dioxide sequestration: Carbon Capture and Storage (CCS) and Carbon Capture and Utilization (CCU), both of which will be investigated in this paper. CCS currently appears to be the more promising approach, as it is relatively well-proven and low-cost compared to CCU. CCU, on the other hand, is growing at a very fast pace and producing many fascinating new processes and technologies, but does not have much of a track record and tends to be prohibitively expensive. Overall, as the worldwide need to cut greenhouse gas emissions (of which carbon dioxide is a major contributor) grows, both CCS and CCU may be viable and necessary options to allow the continued production of energy from fossil fuels while avoiding further greenhouse gas emissions and climate change.

2:00 PM **Balance of System Technologies Under Development to Lower the Cost of Large PV Plants** *Joshua Barrett* (University of Illinois at Chicago)

In this ever-evolving solar technology world, the price per watt continues to decline. It has declined to the point that the photovoltaic panel (PV) is not truly the controlling cost of the end product. Development, site construction, and installation of the product have started to lead in the controlling cost per watt. This paper will examine the overall process of constructing PV farm for central generation, from plant site selection, permitting, environmental concerns, cost of land, framing and mounting systems, maintenance issues, operational costs, infrastructure requirements, grid connection, and end use distribution needs. Though this is a developing technology, large projects have been completed and are operational. We will look at challenges and needs for improvement while reviewing the developing technologies on this subject.

Engineering for Sustainability

Tuesday, March 11, 2014 (Illinois A, **T2D**)

Organizer: *Donald J. Chmielewski* (Illinois Institute of Technology)

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

1:00 PM **CFD Simulation of the Regeneration Process for CO2 Removal using a Regenerable Solid Sorbent** *Emad Ghadirian, S. Zarghami, J. Abbasian and H. Arastoopour* (Illinois Institute of Technology)

Climate Change, which has been associated with the increasing concentration of greenhouse gases (mainly carbon dioxide) is regarded as one of the key environmental issues in the 21st century. Cost effective Carbon Capturing and Storage (CCS) before it is emitted to the atmosphere will result in use of coal and natural gas as the major fuel for electricity generation without affecting economic growth while still reducing carbon emissions to the atmosphere. One of the most promising approaches is use of solid sorbents and fluidized bed process, which currently is not ready for implementation in coal or natural gas based power plants. One of the major challenges is the fact that it is still in the lab or bench scale stages. To successfully scale-up such processes, a powerful tool, i.e. Computational Fluid Dynamics (CFD), is needed to shorten the gap between lab/bench scale and large scales needed for demonstration. Analysis using CFD complements and reduces physical testing, and it can result in a significant time and cost savings while it can give a complete understanding of the processes. Therefore, multiphase Computational Fluid Dynamics (CFD) provides an attractive option to study and design of the gas-solid processes required for continuous CO2 removal using solid sorbents in a systematic and economical way. In this presentation Simulation of Bubbling Fluidized Beds (BFB) for the CO2 removal process will be presented Using kinetic theory based constitutive equations and shrinking core reaction model.

1:30 PM **Mechanistic Modeling of Fast Pyrolysis of Glucose-based Carbohydrates** *Xiaowei Zhou and Linda J. Broadbelt* (Northwestern University)

Fast pyrolysis, a promising thermochemical technology for the production of transportation fuels from lignocellulosic biomass, involves a complex network of competing reactions, which result in the formation of bio-oil, non-condensable gaseous species, and solid char. Bio-oil is a mixture of anhydro sugars, furan derivatives, and oxygenated aromatic and low molecular weight (LMW) compounds. Previously, the successful modeling of fast pyrolysis reactors for biomass conversion was hampered by lumped kinetic models, which fail to predict the bio-oil composition. Hence, a fundamental understanding of the chemistry and kinetics of biomass pyrolysis is important to evaluate the effects of process parameters like temperature, residence time and inorganic slats on the composition of bio-oil.

In this work, we report a mechanistic model that characterizes the primary products of fast pyrolysis of pure glucose-based carbohydrates (glucose, cellobiose, maltohexaose and cellulose). The model incorporates the following condensed phase reactions for the formation of various LMW products in bio-oil: glucosidic bond cleavage, retro-aldol, retro-Diels-Alder, dehydration, hydrolysis, cyclic Grob fragmentation, isomerization and enol-keto transformation reactions. The kinetic rate coefficients were primarily obtained from the literature, based on either experimentally determined Arrhenius parameters for cellulose and model compounds, or theoretically computed values using quantum chemical calculations. A computational framework based on continuous distribution kinetics was constructed to solve the kinetic model. Model results match closely with experimental product distributions from fast pyrolysis of glucose-based carbohydrates over a wide range of pyrolysis temperatures.

The mechanistic model is then expanded to account for the effects of alkali metals, specifically sodium salts, on fast pyrolysis of glucose-based carbohydrates. The modeling efforts to capture the effect of Na+ on the product distribution involved adding interactions of Na+ with cellulose chains and its derivative chains as well as low molecular weight products and adding parallel reaction pathways mediated by sodium ion with altered kinetics into the continuous distribution kinetics model. The requisite kinetic parameters were obtained by using density functional theory calculations and transition state theory. The model, utilizing the same set of rate coefficients, is able to predict the yields of various products from fast pyrolysis of glucose, cellobiose, maltohexaose and cellulose that also are in good agreement with experimental data over a wide range of Na+ concentrations.

2:00 PM **Bifurcation Analysis of Wastewater Treatment Operation** *Mustafa Cagdas Ozturk, Arun Kumar Raju Ganesan, Paul R. Anderson, Fouad Teymour* (Illinois Institute of Technology)

Wastewater treatment plants (WWTPs) require large amounts of energy owing to the forced aeration in the activated sludge process. Aeration plays a critical role in the process, such that, it maintains proper biomass activity, increases the dissolved oxygen content of the water and enhances mixing. In most WWTPs, the rate of aeration is kept at unnecessarily high levels. This is done to render the plant resilient towards upstream disturbances, which may otherwise deteriorate the discharge quality and result in violation of the strictly monitored discharge permits. In such a case, however, a better remedy would be a control scheme which can adjust the aeration rate in accordance with the disturbances and process conditions. Undoubtedly, this requires a good understanding of the complex behavior of such a process, which, along the way would yield a more cost-effective operation.

Mathematical modeling offers deep insight into the workings of a process, especially when coupled with a bifurcation analysis approach, as we present in this study. A complete bifurcation analysis enables the classification and quantification of the entire operating space, thus allowing for a global view of operational constraints and risks. In that respect, it can help create decision tools and pathways for controller design. Such insight becomes especially valuable for designing intelligent systems such as agent based controllers.

This bifurcation study focuses on Stickney Water Reclamation Plant (WRP) in West Chicago, which is the world's largest WWTP. We use a recently developed model of the Stickney WRP, which was validated with historical data from the plant from 2001 to 2009. The process is modeled as a 1-D continuous reactor (discretized as a train of 48 CSTR tanks) followed by a settler/clarifier with return activated solids recycling. The kinetic model is based on the widely used Activated Sludge Model no. 1 (ASM1). A custom continuation algorithm was used to carry out the bifurcation analysis on the resulting 480 algebraic (originally ordinary differential) equations. Attention was given to effluent concentrations of ammonia, dissolved oxygen and the biomass in evaluating the analysis results. This is the first instance of a bifurcation analysis of such a comprehensive model for the activated sludge process. Previous studies were limited to simplified models that were not validated against existing installations. When the total wastewater flow rate into the plant was used as a bifurcation parameter, multiple steady states can be broadly located, even in the vicinity of the nominal flow rate used by the process. The steady state set consists of a steady state where the coexistence of two biomass species (autotrophic and heterotrophic) is possible, states where only heterotrophs or autotrophs can exist, and a washout steady state at which no biomass exists. This finding has important implications on the operation of the WWTP. Similar observations are made when ammonia loading and water temperature are considered as bifurcation parameters.

We also used the bifurcation approach to analyze the behavior of the plant during major storm events that result in sustained increased inflow owing to the nature of the combined flow situation into the sewer network of Chicago and most major cities. The results show that permit violation may occur during the long transients of storm events. Possible remedial actions are proposed.

One chief aim of this study was the assessment of air usage at different conditions; hence a bifurcation analysis on airflow was performed indirectly by varying the mass transfer coefficient of dissolved oxygen. Results show that it is possible to reduce the airflow by about 40-60% of the nominal value, without causing an increase in ammonia or a decrease in dissolved oxygen. This represents significant energy savings for this process. Therefore, it is possible to achieve the sustainability goals of WWTPs, if proper control strategies are implemented. We are currently working on encapsulating the knowledge gained from the bifurcation study into an Agent-Based system (ABS) for monitoring and control of the cyber-physical system resulting from the combination of the treatment process, a sensor network, and the ABS.

YP Mock Interviews

Tuesday, March 11, 2014 (East Terrace and Monarch, **T2E**)
Organizer: *Julie Gruhn* (UOP)
Chair: *Abigail Jackson* (Tetra Pak)

1:00 PM (Monarch) **Relax - It's just an interview** *Julie Gruhn* (UOP)

Tips and tricks on how to be prepared to put forward your best self for the interview for the job you want. After the presentation the interview team will be available for one on one consultation and practice interviews. Please bring a copy of your resume to interviews.

1:30 (East Terrace, floor 2) **Mock Interviews**
Julie Gruhn (UOP), *Abigail Jackson* (Tetra Pak), *Jerry Wilks* (CITGO), *Jeremy Isaacs* (Middough), and *Todd MacMillan* (Ecolab)

Corn to Chemicals Industrial Complex I

Tuesday, March 11, 2014 (Illinois B, **T2F**)
Organizer and Chair: *Jeffery P Perl* (University of Illinois at Chicago and Chicago Chem Consultants)

1:00 PM **UIC Senior Process Design - "Corn to Chemicals"** *Jeffery P Perl* (University of Illinois at Chicago and Chicago Chem Consultants)

Every spring, for the past 6 years, a new design problem is posed to our seniors. This year, a total of 43 students have been split into 10 teams, each having an industry client / mentor. This year's project, "Corn to Chemicals" was originally suggested by Jim Foster and Chris Hofmann, both of Archer

Daniels Midland (ADM), Decatur Illinois. Additional input was obtained from our mentor group to produce a suitable, unified, industrial concept problem. The student teams each have distinct, recognizable unit operations that in total comprise a modern fully mass and energy integrated complex. Every three weeks, each team makes a 25 minute presentation to all groups and mentors. These project progress reports are used to tune-up as well as move forward towards developing a stage gate 1 preliminary design and cost estimate, much as it is done at Ambitech, Middough, Jacobs and UOP from whence our mentors are drawn. The 10 projects are well under way and is the third review meeting, which you are welcome to both attend and participate in as well. Please join us.

1:05 PM **Corn Germ Utilization: Corn Oil Extraction, Refining, and Biodiesel Production via Supercritical Transesterification** *Jack Blachut, Kunal Gulati, Monika Jonuskeviciute, Paul Schoeneck* (University of Illinois at Chicago) *and Dan Rusinak* (Middough)

The rapid growth of fuel ethanol has increased the agricultural development of corn, thereby increasing the supply of byproduct corn oil from the germ portion of the corn kernel. With a surplus of corn oil and a diminishing fossil fuel oil supply, support for alternative fuel sources is rising. Correspondingly, a Federal mandate has pushed for higher non-petroleum blends in fuel; this has opened a vast market for biodiesel. Biodiesel is becoming the most practical alternative fuel source due to its compatibility with existing diesel engines and environmentally friendly emissions profile. Perhaps the biggest benefit of biodiesel is the capability of domestic production from non-petroleum and renewable resources. Although biodiesel production from vegetable oil is well established, the catalyzed processes commonly used today presents a series of limitations and drawbacks due to high energy costs required for long reaction times and complicated biodiesel purifications. The biodiesel manufacturing in this design utilizes a supercritical non-catalyzed transesterification – a new and potentially lucrative method of biodiesel production. This design leads to quicker and higher biodiesel yields due to conversion of free fatty acids, therefore, simplifying the post-purification process.

The design goal of this process is to economically and efficiently extract, refine and produce biodiesel from corn germ, with minimal negative impact on the environment. The production of biodiesel through the extraction and refinement of the crude corn oil is virtually a waste free process as all of its byproducts hold economic value from the food industry to the pharmaceutical industry. With the use of the non-conventional process of supercritical transesterification, a shorter reaction time as well as a higher yield is achieved. This process provides an interesting alternative to a cleaner, more efficient and versatile method of biodiesel production, resulting in optimization of industrial biodiesel production.

1:30 PM **Corn Receiving and Steeping Process** *Patrick Coan, Andre Colorina, Alan Reusnow, Jana Rush, Molly Sompolski* (University of Illinois at Chicago) *and John Micheli* (Middough)

Recent advances in corn production have allowed for essentially complete conversion of corn into valuable products, including oils, low weight polyols, and low-weight alcohols. Before these products can be made, however, shelled corn must first go through a wet milling process. The wet milling process is designed to separate corn into its components of starch, germ, gluten, and fiber, each of which can then be converted to sellable products. Consequently, there is a continuing need for an initial steeping process to soften the corn and begin the separation process. Before steeping, corn is cleaned to remove foreign materials. Molten sulfur is burned and the resulting sulfur dioxide is absorbed into water to produce a dilute sulfurous acid solution that controls microbial growth. The steeping process consists primarily of soaking the corn in the dilute sulfurous acid for 36 hours using a batch-continuous method. The process is capable of steeping 100,000 bushels of corn per day. Steeped corn is then sent to a germ separation process. The steeping liquor containing dissolved and suspended solids is concentrated into heavy steep water and added downstream into the fiber or gluten dryer feeds as a nutrient component of animal feed products. Our goal is to design a process that maximizes the potential for downstream separation, while minimizing costs. Although the Corn Receiving and Steeping Process will not produce any finished products, it is designed to be the first part of a larger Integrated Corn Production Complex, and is essential to the Complex's overall success.

1:55 PM **Combined Heat and Power for Corn Wet Milling** *Kunal Desai, Roberto Gomez, Mike Kramer, and Paulina Mlynarska* (University of Illinois at Chicago) *and Dave Bahr* (Jacobs Consultancy)

This plant allows for the recovery and purification of corn based food and chemical products. The demand for these products is high as they can be used in a variety of ways including food, feedstock, and fuel. The heat and power requirements for the facility are electricity and steam. Hydrogen, cooling water, and instrument quality compressed air will also be provided. The combined cycle power plant combusts natural gas generating electricity as the gas is expanded through a gas turbine. The exhaust out of the gas turbine contains a lot of energy allowing it to be used to generate high-pressure process utility steam. Conventional power plants lose this heat energy, but here the "waste" steam is expanded through a steam turbine generating additional electricity and meeting the heat demands. This combined heat and power block helps avoid a negative net present value, as it utilizes waste heat. Bi-directional grid connectivity will allow excess electricity to be sold at a profit to further optimize value through a balanced use of natural gas and electricity as these commodity prices change. Steam methane reforming provides

a cost effective solution for satisfying the hydrogen demand. Methane and steam react in the steam methane reformer yielding carbon monoxide and hydrogen. In a water shift reaction, carbon monoxide is reacted with water to form carbon dioxide and additional hydrogen that is separated out through a pressure swing adsorption. Water is cooled by evaporation into air in a cooling tower providing cooling water.

2:20 PM **Sorbitol and Dextrose Production from Corn Starch** *Taras Dykun, Ricardo Plascencia, Patty Rottinghaus, Sarah Wiersema* (University of Illinois at Chicago) *and Tom Stephan* (Consultant)

The corn wet milling process is used to separate corn into its four main components: starch, oil, gluten, and fiber. The largest component, starch, can be converted into a variety of products, one of which is dextrose. In this process, the conversion of starch to dextrose is performed by treating diluted starch with enzymes such as α-Amylase, Gluco-Amylase, and Pullulanase. The dextrose will then be converted into sorbitol via hydrogenation. Our primary goal is to maximize profit and minimize losses in a plant such as this where 100,000 MTY of sorbitol is to be produced; we also aim to comply with environmental, safety, and occupational health regulations. Our process consists of four main steps: gelatinization, liquefaction, saccharification, and hydrogenation. Gelatinization is the process of breaking down the intermolecular bonds of the starch molecules in the presence of water and heat. Liquefaction occurs when alpha amylase enzymes are added to break down the gelatinized starch. Saccharification occurs when glucoamylase and pullulanase enzymes are added to break down the solution further, creating a dextrose solution. The dextrose solution will then be purified and sent to the hydrogenation process where a powdered Nickel catalyst will be added to the solution. The mixture will then be sent to a continuous stirred tank reactor in order to produce sorbitol. To minimize waste, the nickel catalyst and excess hydrogen are removed from the sorbitol product stream and reused. Therefore, this design allows for the production of sorbitol with maximum purity and minimum waste.

Hydraulic Fracturing – Process Overview and Implementation, Water Management, and Impact on Illinois Economy

Tuesday, March 11, 2014 (Cardinal Room, **T3A**)

Organizer and Chair: *Jordan Ciezobka* (Gas Technology Institute)

3:00 PM **Hydraulic Fracturing – Old Technology in New Places: Process Overview and Technology Evolution** *Jordan Ciezobka* (Gas Technology Institute)

Hydraulic Fracturing is a technique used to enhance permeability in oil and gas bearing formations. Since it was first applied in the 1940's, it has played a vital role in increasing U.S. energy production, especially from low permeability formations such as tight sands and shales. Hydraulic fracturing and the discovery of many new productive shale oil and gas formations has made the U.S. the largest natural gas producer in the world and is now enabling increases in oil production. Hydraulic fracturing has created good paying jobs, contributed toward reducing the cost of energy to consumers, increased energy security, reduced CO2 emissions (by displacing coal for power generation), and may potentially revitalize the competitiveness of the manufacturing base (by lowering fuel and feedstock costs). However, this industrial activity has also expanded toward large metropolitan areas and has brought the technology to people's back yards, literally. We'll explore the evolution of hydraulic fracturing technology and discuss why it is needed for commercial gas production while considering safety of the fracturing process and the current monitoring techniques.

3:30 PM **Issues and Challenges in the Management of Flowback Water and Solid Wastes Associated with Shale Gas Development** *Tom Hayes* (Gas Technology Institute)

A necessary step for the release of natural gas from shale rock in most shale gas plays is the procedure of hydraulic fracturing which involves the pumping of about 4 million gallons of water plus additives into a horizontal well followed by the collection of a portion of the injected water stream (regarded as a "flowback" water). This flowback contains salts, oils & greases, BTEX, polymer (slick water constituent) and heavy metals. This presentation will summarize water characterization, discuss the environmental issues associated the life cycle of a typical shale gas development area, and will describe the results of an engineering analysis treatment options for shale gas brines. In the field, the natural gas industry is evaluating a number of water processing approaches to facilitate flowback water reuse and responsible produced water management. Some of these leading treatment approaches are aimed at the demineralization of shale gas water streams. The economics of various water management options will also be discussed. Options for drill cuttings and solid waste management (including beneficial use) will also being discussed.

4:00 PM **Hydraulic Fracturing in Illinois - Will it work and what could it mean for Illinois' economy?** *Tom Wolf* (Illinois Chamber of Commerce)

Illinois has passed legislation specific to hydraulic fracturing. But the devil is in the details. Tom Wolf, the executive director of the Energy Council will provide background on the new regulations, the on-going rulemaking process, the continuing political situation, the attitudes of the producers and what it all could mean for job development in Illinois.

Engineering Cellular Cardiology

Tuesday, March 11, 2014 (White Oak AB, **T3B**)

Organizer and Chair: *Katherine Sheehan* (DePaul University)

3:00 PM **Cardiac Tissue Repair by Local Delivery of a Growth Factor from Polymeric Microrods** *Brenda Russell and Golnar Doroudian* (University of Illinois at Chicago)

Local release of drugs for tissue repair is a major challenge. Bioengineering approaches allow microstructures to be fabricated that contain bioactive peptides for local delivery. Heart tissue damage is associated with local increases in Mechano Growth Factor (MGF-E), which may recruit local stem cells to participate in myocardial repair. Microrod delivery devices were fabricated of poly (ethylene glycol) dimethacrylate (PEGDMA) hydrogel and loaded with MGF-E domain peptide in order to determine the elution profile and bioactivity. The microrods were 15 μm by 100 μm with 30 kPa stiffness. The MGF delivered from microrods blunted proliferation of human mesenchymal stem cells and reduced apoptosis of neonatal rat heart cells subjected to hypoxia. Thus, MGF-loaded microrods injected into injured mouse heart may improve cardiac function.

3:25 PM **Rescue of Familial Cardiomyopathies by Modulation of Ca2+ fluxes and Myofilament Response to Ca2+** *Beata M. Wolska* (University of Illinois at Chicago)

Cardiomypathies are a heterogeneous group of diseases of the myocardium associated with hemodynamic and/or electrical dysfunction and they frequently show an inherited character. Familial cardiomyopathies include hypertrophic cardiomyopathy (HCM), dilated cardiomyopathy (DCM), restrictive cardiomyopathy and ventricular noncompaction cardiomyopathy. These inherited cardiomyopathies are cased by mutations in several genes encoding sarcomeric proteins. HCM typically involves increased myofilament Ca2+ sensitivity associated with diastolic dysfunction, whereas DCM often results in decreased myofilament Ca2+ sensitivity and systolic dysfunction. In addition to alterations in myofilament Ca2+ sensitivity, alterations in the levels of Ca2+-handling proteins have also been described in HCM and DCM. Our recent work with mouse models of HCM and DCM showed that they can be rescued via modification of myofilament Ca2+ sensitivity and by altering Ca2+ homeostasis by targeting Ca2+-handling proteins, such as the sarcoplasmic reticulum ATPase and phospholamban. Our data strongly indicate that bringing the myofilament sensitivity to Ca2+ closer to normal levels or intervention in Ca2+ regulation can delay or prevent development of HCM and DCM and should be considered as therapeutic targets for these diseases.

3:50 PM **p21-activated kinase-1 signaling alters atrial excitation contraction coupling (ecc)** *Katherine Sheehan* (DePaul University)*, R. John Solaro, Beata M. Wolska* (University of Illinois at Chicago)

Contractile function in the heart is regulated by a number of kinases and phosphatases, making them attractive potential drug targets to treat cardiac disease, yet their mechanisms of action are not completely understood. Atrial arrhythmias are a growing public health problem but the lack of atrial-specific knowledge of the signaling pathways involved in arrhythmia onset and their effects on cellular protein function limits development of effective pharmacological therapies. p-21-activated kinase-1 (PAK1) is an attractive potential candidate. A serine-threonine kinase recently discovered in cardiac myocytes, PAK1 activates protein phosphatase 2A (PP2A) and attenuates the effects of ß-adrenergic stimulation on the intracellular Ca2+ transient, and the membrane ion currents ICa,L, and IKr, In a model of electrically paced isolated rat atrial myocytes PAK1 activation combined with ß-adrenergic stimulation induced a loss of fidelity of beating to stimulus, indicating altered function of Ca2+ flux proteins. Current experiments will determine the specific protein changes. We anticipate this cellular model will allow the identification and testing of molecular signaling targets for potential drug development.

4:15 PM **Synthesis and Characterization of Phosphate-Loaded PEG Diacrylate Hydrogel Nanoparticles by Inverse Miniemulsion Polymerization** *Srivishnu Vadlamudi, Fouad Teymour, Georgia Papavasiliou* (Illinois Institute of Technology)

Drug delivery is an exciting field of interdisciplinary research that has captured the interests of the Pharmaceutical and Biotechnology industry. With the continual advances in discovery and synthesis of effective drugs, it is imperative to create safe and efficient drug-delivery systems. Biocompatible polymer nanoparticles are beginning to provide innovative solutions and form the frontier of advanced drug-delivery technology and Nanomedicine.

Phosphate ions have been identified to be instrumental in healing wounds and preventing post-surgery gut-derived sepsis. We have developed a process of inverse miniemulsion polymerization to produce highly crosslinked, Biocompatible PEG Diacrylate nanoparticles in the size range of 150-250 nm and comprising phosphate ions.

An aqueous solution containing high amounts of crosslinker (PEG Diacrylate 575), NVP, phosphate salt and a water-soluble thermal initiator was emulsified in cyclohexane (oil-phase) by the application of high shear (ultrasound) to generate an inverse miniemulsion. The aqueous nano-droplets were stabilized against coalescence by the use for two non-ionic surfactants. The presence of phosphate salt within these stable nano-droplets prevented destabilization of the miniemulsion against Ostwald ripening. The encapsulation of phosphate within the nanoparticles is made certain by selecting a phosphate concentration dictated by the PEGDA-Phosphate temperature-dependent thermodynamics. Reported experimental measurements include monomer conversion, particle size measurement and aqueous swelling characteristics. Nanoparticle tracking Analysis (NTA) methodology developed by *Nanosight* was used for particle size measurements. A factorial design of experimentation coupled with the application of a kinetic model indicate a low range (10^{-3} – 10^{-4}) of the initiator efficiency in the reaction

kinetics. The comparison of experimental conversion data with model predictions, points towards a well documented notion of a drastic reduction in initiator efficiency once a critical degree of crosslinking is achieved within the nanoparticles, during the reaction. The inverse swelling ratios (analogous to crosslink density) of the purified nanoparticles tend to substantiate the above kinetic behavior. The preliminary medical testing of the synthesized nanoparticles showed promising results indicating the efficacy of this strategy in nanomedicine.

Issues in Emerging Energy Technologies II

Tuesday, March 11, 2014 (Fort Dearborn B, **T3C**)
Organizer and Chair: William Ryan (University of Illinois at Chicago)

3:00 PM **Mitigation Strategies for Beyond Design Basis External Events** *Sandra Parker* (University of Illinois at Chicago)

The earthquake and tsunami that caused a nuclear accident at Tokyo Electric Power Co.'s Fukushima Dai-ichi nuclear power plant in Japan on March 11, 2011 has raised worldwide attention regarding nuclear safety. As a result of this disaster, the U.S. Nuclear Regulatory Commission developed a Task Force to review U.S. nuclear regulations related to mitigating and responding to a similar accident in the U.S. This paper discusses the regulation changes that were invoked on U.S. nuclear power reactor licensees based on the Fukushima lessons learned and how these changes positively affect the way U.S. nuclear plants will mitigate, prevent and respond to emergencies resulting from extreme events. Specifically, the paper details the three phase approach and requirements that U.S. NRC Order EA-12-049 has placed on U.S. nuclear power facilities to implement diverse and flexible coping strategies called FLEX.

3:20 PM **Energy Performance Contracting** *Wildivina Rosario* (University of Illinois at Chicago)

As facilities begin to age and equipment to deteriorate over time, there is a growing need for comprehensive solutions that address the demands for improvement at little to no costs. Energy Performance Contracting (EPC) offers a guarantee on performance-based solutions that allow the customer to perform facility improvements, which are funded through energy savings. The purpose of this paper is to describe and provide an overview of the EPC program. It covers the history of EPC; from its beginnings in the 1970s to its current status of being the main tool used in the public sector for efficiency projects. It also covers the EPC market including constraints and drivers that help shape the business. One of the main differentiators of EPC is the financial offering and the ability to guarantee the savings through measurement and verification. Both the financing and the measurement and verification topics are further detailed in the report along with a section on the future of EPC and some of the benefits that it provides the customer.

3:40 PM **Wave Energy Converter Technology** *Greg Studier* (University of Illinois at Chicago)

Energy use around the world is expected to continue expanding at a dramatic rate for the foreseeable future, even with continued improvements in efficiency. The U.S. Energy Information Administration has projected that there will be a 56 percent increase in energy consumption between the years 2010 and 2040 [1]. This astounding increase in the amount of energy the world needs to produce will have to be met with increasingly sustainable forms of generation as well. Greenhouse gas emissions continue to grow almost unabated, with CO2 concentration rising over 390 ppm in 2010; this represents a 39% increase above preindustrial levels [2]. To avoid the worst possible effects of climate change, this increase in emissions must be curbed. Looking to renewable forms of energy is the most obvious way to accomplish this goal. Enormous interest in wind and solar energy has resulted in them playing an increasing role in energy production worldwide. However, absent a new and affordable way of storing electricity, wind and solar energy cannot hope to displace fossil fuel and nuclear generation in a significant way due to their intermittent nature. The potential to exploit a more consistent form of renewable energy – ocean wave energy – will be the focus of this paper. Presented will be an overview of wave physics, equations, formation, and propagation; the power take off methods utilized; the classification of the different types of wave energy converter (WEC) technologies, and a survey of the most commercially viable designs.

4:00 PM **Performance of Hybrid Solar Photovoltaic Thermal Collectors** *Jerad Tintera* (University of Illinois at Chicago)

Much research is devoted to finding low cost ways to improve the performance of traditional photovoltaic cells (PV). Hybrid solar photovoltaic thermal (PVT) collectors are a technology that simultaneously extracts electricity and thermal energy from the sun. Due to temperature sensitivity of the semiconductor material used in PV cells, PVT actually increases the efficiency of these cells by extracting heat and lowering the cell temperature. In addition to increased electricity output, useful thermal energy is generated, thus increasing the overall efficiency of the collector. The synergy between PV cells and thermal collectors means that a typical PVT system has a higher overall efficiency than separate PV and thermal systems combined. In this paper we will review the theoretical performance of PVT collectors. In addition some experimental and real-world results will be examined.

YP Conflict Resolution Panel

Tuesday, March 11, 2014 (Illinois A, **T3D**)
Organizer and Chair: *Julie Gruhn* (UOP)

3:00 PM **Resolving Conflict in the Workplace** *Taylor Newsom* (BP), *Jerry Wilks* (Citgo), and *Todd MacMillan* (Ecolab)
This session features a panel discussion on how to avoid and resolve conflict in the work place and best practices for professional communications.

Corn to Chemicals Industrial Complex II

Tuesday, March 11, 2014 (Illinois B, **T3F**)
Organizer and Chair: *Jeffery P Perl* (University of Illinois at Chicago and Chicago Chem Consultants)

3:00 PM **Corn Wet Milling Germ Separation** *Will Abbott, Justin Barak, Meghan Lapeta, Jong Shin, Sandy Younan* (University of Illinois at Chicago) *and Shannon Brown* (Ambitech)
Corn wet milling has been around for a long time, over 150 years in fact, yet it can still be quite inefficient. Corn wet milling is the most energy intensive of all food industries and consumes fifteen percent of all energy usage in the entire food industry. In the corn wet mill, the germ separation and drying unit accounts for seven percent of the energy used. Since a single corn wet mill can spend upwards of $30 million per year on energy costs, energy efficiency is paramount in allowing continued competitiveness. With these motivations in mind, we designed a germ separation process unit, which is a necessary component of a corn wet mill, to be as energy efficient as possible. We accomplished this through effectively using so-called waste heat to preheat streams as possible and squeeze the most amount of energy out of process streams while minimizing unrecovered heat and heat losses. Furthermore we take all environmental concerns into consideration to ensure adherence to federal and state regulations. At this stage of design, the project was designed through a stage gate one analysis including payback period and ROI with our recommendation to build the plant.

3:25 PM **Corn Wet Milling Second Grind and Fiber Drying** *Anwar Beker, Leidy Nallely Jimenez, Katarzyna Orbik, Collin Pearsall, Elizabeth Wanic* (University of Illinois at Chicago) *and Jerry Palmer* (Ambitech)
In order to facilitate sustainable growth, the chemical industry needs to shift from productions based upon fossil fuels to more sustainable material sources. This project seeks to shift material sourcing from traditional oil to corn in the production of biodiesel from corn oil. Utilizing corn in this process will require wet milling to separate the grain into high value starch, protein, fiber, and other products. Specifically, this project will design by simulation an economical and environmentally sound process for extracting a slurry of starch and gluten protein from corn. The design will fit into a facility which processes 100,000 bushels of corn per day and will produce animal feed from the corn fiber, steep-water liquor, de-oiled germ, and other byproducts within the plant. Primary operations in this part of the processing plant, known as the second grind, will employ milling and grinding, screening and washing, dewatering and drying, and, if needed, pelletizing

3:50 PM **Reactor Design for Polyols Production** *Ryan Rock, Nathan Liebmann, Andrew McNamara, Elmar Reyes* (University of Illinois at Chicago) *and Bill Keesom* (Jacobs Consultancy)
Glycols are one of the most widely sold chemical merchant products in the world. Millions of metric tons per year of propylene glycol are sold worldwide to manufacture antifreezes, food additives, pharmaceuticals and various other chemicals used in industry. The current mode of manufacture is from the byproducts of petroleum refinement. However, as petroleum resources begin to dwindle the environmentally friendly production of glycols from renewable materials will become more and more competitive. As a result, there is a great opportunity for companies in the U.S. to utilize corn as a raw material to produce glycols – and by extension remain a global leader in the chemical marketplace. The process that we have explored here does exactly this. Sorbitol made from corn is used as a feedstock to generate propylene and ethylene glycols as well as several other byproducts that can be sold on the market. In order to make these products the choice of catalyst and the design of both the reactor and the ancillary equipment all had to be taken into careful consideration. The end result of this work is an eco-friendly glycols production process that will play a vital role in keeping the U.S. ahead in the chemical manufacturing industry for years to come.

4:15 PM **Polyols Separation** *Amber May, Steven Priest, Daniel Sobieski, Garrett Youngblood* (University of Illinois at Chicago) *and Dennis O'Brien* (Jacobs Consultancy)
In an effort to reduce the consumption of fossil fuel, many manufacturers are seeking ways to increase the renewable content of their products. Glycols are among these products. Two of the main glycol commodities are propylene glycol (1,2-propanediol; $C_3H_8O_2$) and ethylene glycol ($C_2H_6O_2$). These are used in anti-freezes, pharmaceuticals, personal care products, and foods. Both are widely used as intermediates for the synthesis of other chemicals such as polyesters and polyurethanes. Through the hydrocracking of sorbitol (sugar alcohol produced from a corn feedstock), a biobased polyol mixture of over 50 compounds and isomers is created. Separation of propylene glycol and ethylene glycol from this complex polyol mixture is challenging due to the proximity of the polyol components' boiling points and solvency. Currently, many methods and patents have been developed for the hydrocracking process. These have not been developed on a commercial scale because the processes for separating the resultant compounds produced are complex and expensive. The goal of this team is to design a process that separates propylene glycol, ethylene glycol, and alcohols from a complex

polyol stream. The process incorporates ordinary distillation, extractive distillation, membranes, and other technology to find the lowest cost methods to purify the desired propylene glycol and ethylene glycol products to a technical or USP quality grade equivalent to petrochemical-based glycols.

4:40 PM **Water Treatment Facility in Corn Wet Mill Plant** *Mark Hartman, David Hu, Christopher Rebolloso, Ethan Rendlen* (University of Illinois at Chicago) *and Patrick Shannon* (Middough)

Ethanol production from corn is a growing market that is reshaping the fuel industry by reducing the demand of crude oil the U.S. The corn to ethanol process requires a substantial amount of water at varying purities. The use of corn in the production of ethanol has been controversial issue due to its energy and water consumption. With rigorous environmental regulation, lack of water availability, and economic benefits of water reuse, this facility will aim to be a zero liquid discharge (ZLD) facility. ZLD eliminates wastewater effluent into waterways which can negatively impact the nearby ecosystem. As well as reducing the amount of intake water to the facility and in some cases recovering valuable by-products. Utilizing modern anaerobic water treatment technology the facility will produce biogas, which used as fuel, will reduce the net energy requirements of the entire process. The anaerobic treatment will significantly reduce the amount of organic contaminants and in combination with ultrafiltration, softening and demineralization processes produce clean reusable water for the corn wet mill complex. The plant will be capable of implementation of additional waste to energy sources such as surrounding sanitary and farm waste if desired. Some solid waste can be reused as fertilizer, increasing the symbiotic relationship of the process with the surrounding rural area. Overall, this water treatment facility will substantially reduce the environmental concerns revolving water usage in a corn wet mill plant, while providing the plant with clean, reliable, and cheap water.

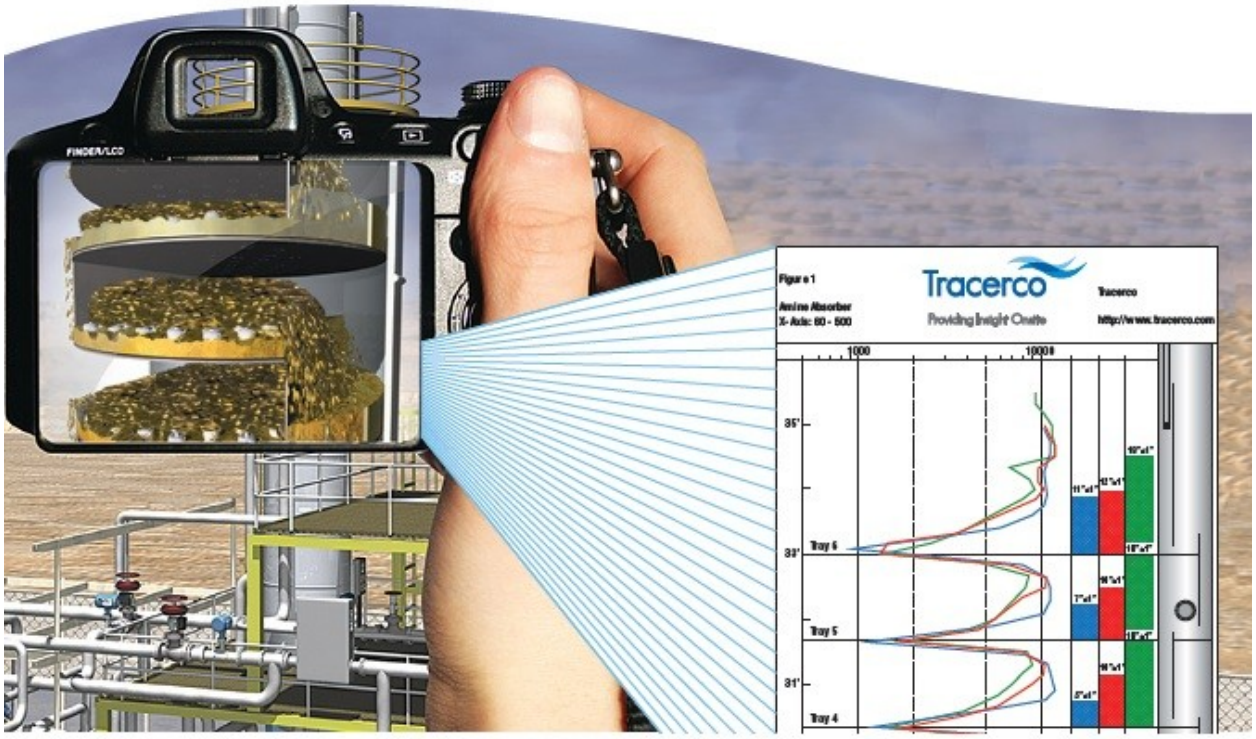
5:05 PM **Centrifugal Separation of Starch and Gluten** *Osman Braimah, Mike Nguyen, Ishai Strauss, James Walsh* (University of Illinois at Chicago) *and Jerry Palmer* (Ambitech)

Corn Wet Milling is a corn refining process in which corn is separated into its various components, namely starch, oil, gluten, and fiber. This process yields numerous products and byproducts, which are used in a variety of applications from pharmaceuticals to food processing to animal feeds. On an industrial scale, the process of Corn Wet Milling becomes complex, costly, and energy intensive. For our project, we were given a portion of the Corn Wet Milling process, specifically starch and gluten separation and drying. The task was to use our engineering knowledge to design a reasonable, efficient process for separating and drying starch and gluten generated from 100,000 bushels per day of corn, which would then be used by subsequent groups to produce animal feed, pharmaceutical feedstock, and other profitable products. Requirements that were taken into consideration were the ability to justify our reasoning for particular process equipment, following EPA regulations, and producing enough starch to meet the design specification for conversion into dextrose and sorbitol. Throughout the process of this project, a detailed mass and energy balance was maintained as well as researching various competing processes and potential products that could be produced to maximize profit.

Onsite Tray Capacity Diagnostics Using TRACERCO FrothView™ Technology

Tracerco

Providing Insight Onsite



A new dimension to tower scanning tray analysis

Patent pending TRACERCO FrothView™ technology is now being used to measure capacity of trays in separation towers. A combination of field data gathering improvements together with sophisticated density profile analysis allows instant reporting of tray froth height, expressed as % tray space. Extensive pilot plant studies have verified that TRACERCO FrothView™ corresponds well to the % flood of an operating tray. To learn more about our unique tray analysis contact a technical advisor in your area to schedule a presentation.

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Process Diagnostics

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7th Annual AIChE Midwest Regional Conference

Illinois Institute of Technology

Spring 2015

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

Young Professionals Social

Come and join your fellow YP's in celebrating a successful conference by relaxing at the YP Social for networking, drinks, and great conversation! Feel free to join us even if you weren't able to make it to the conference!

What: YP Social after the 6th Annual Midwest Regional Conference @ UIC
When: Tues, March 11, 5:30PM – 8:30PM
Where: Morgan's on Maxwell St
1325 S. Halsted St
Chicago, IL

Soft Drinks and Appetizers Provided by AIChE Chicago
Hosted by AIChE Chicago Young Professionals Committee (YPC)