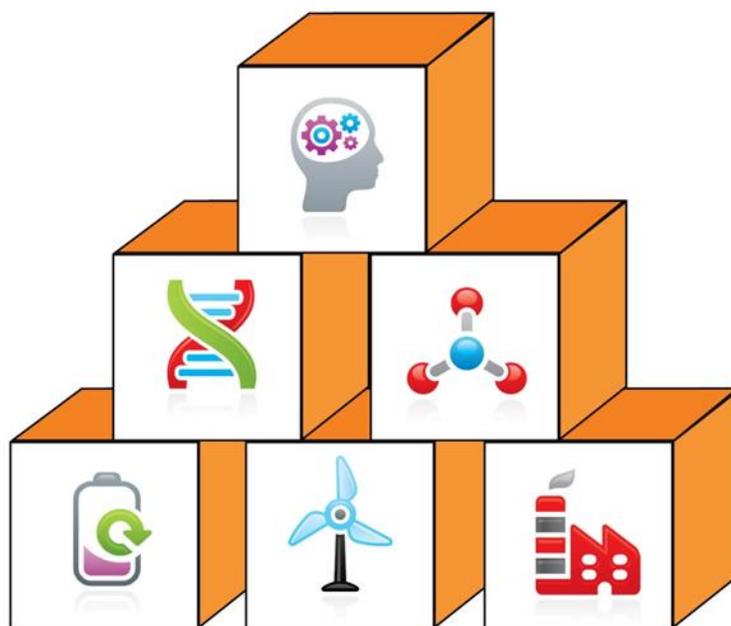


# AIChE 2010

Midwest Regional Conference  
September 30 - October 1 | Chicago, Illinois

## Building the Future of Chemical Engineering



Nanotechnology | Pharmaceuticals | Process Engineering

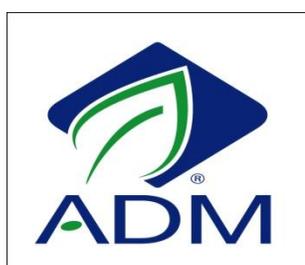
Energy Generation and Renewables | Biological Engineering

Presented by the AIChE Chicago Section

Hosted by  ILLINOIS INSTITUTE OF TECHNOLOGY

## Conference Sponsors

We would like to thank our 2010 AIChE Midwest Regional Conference Sponsors. This conference would not be possible without their support.



[ WANGER INSTITUTE FOR SUSTAINABLE ENERGY RESEARCH ]  
AT ILLINOIS INSTITUTE OF TECHNOLOGY

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## Introduction

In its 3<sup>rd</sup> consecutive year, the AIChE Midwest Regional Conference promises to boost your professional career and will prepare you to take your organization in new directions. By way of the Chicago Local Section, AIChE headquarters support and Illinois Institute of Technology, the conference will provide the opportunity for engineers and scientists in the region to learn about new technologies, as well as offering an engaging atmosphere for networking.

This year's conference continues to focus on the critical subjects of energy and sustainability, as well as other key areas that impact the Midwest region. The areas of particular focus are the following: Energy and Renewables, Environmental Health and Safety, Process Development, Refining, Sustainability and Pharmaceuticals.

Conference highlights include:

- Thursday Keynote Speaker: **Bill Hoback**, Office of Coal Development, Springfield, IL
- Friday Keynote Speaker: **Maria Burka**, Program director of Process and Reaction Engineering in the Chemical, Bioengineering, Environmental, and Transport Systems Division of the National Science Foundation
- Thursday Evening Poster Session: which features topics of interest in chemical engineering research and development.

Additionally the Chicago Local Section, along with the Illinois Institute of Technology is pleased to continue sponsoring the High School Engineering Career Outreach Program. The program allows Chicago-area high school students to become acquainted with the various facets of the chemical engineering profession. The program will take place on both days and the featured speaker is former NASA payload specialist and current professor of chemical engineering at Northeastern University, **Dr. Al Sacco**. The program also includes a special luncheon where students can interact with practicing chemical engineers.

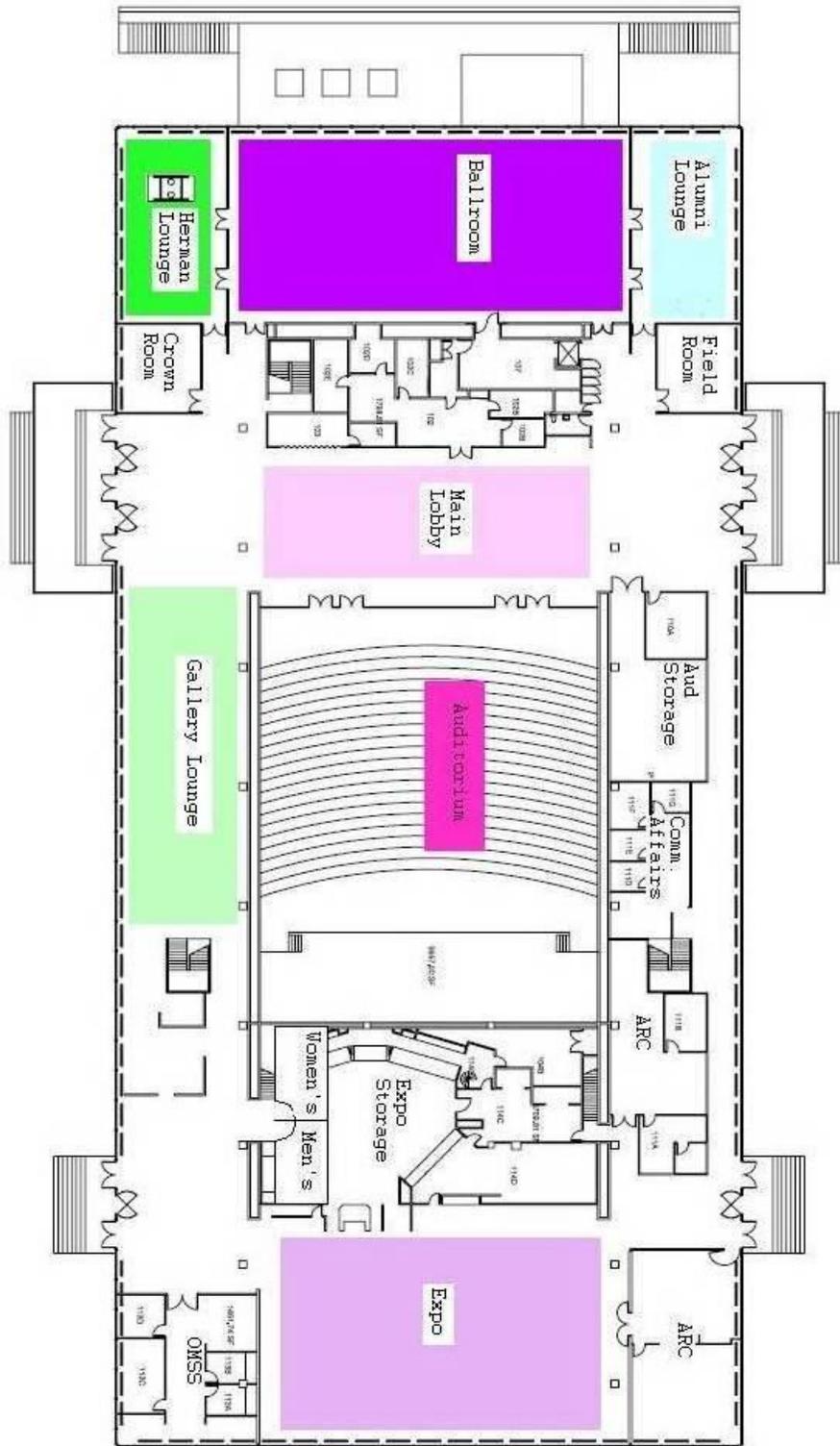
For young professional engineers, there will be a number of workshops held on both days to help fine-tune interviewing skills, improve the effectiveness of resumes and allow for social networking opportunities.

Please look at the inside front cover of this program book as well as our website, <http://www.aiche.org/Conferences/2010chicagoconference.aspx>, to see the many corporate sponsors who helped to make this program possible, both through financial assistance and the time their staff spent helping and attending the programs.

**Welcome, from the 2010 Symposium Organizing Committee.**

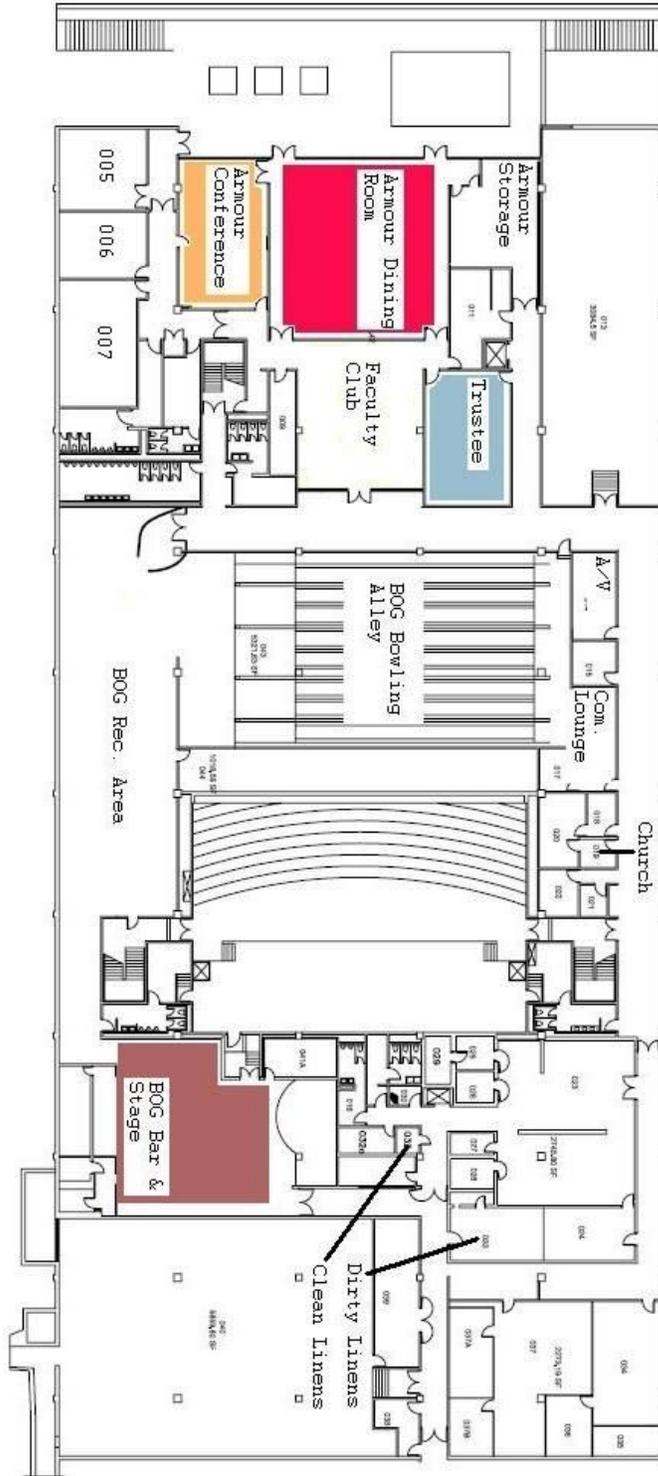
# Map of Main Level

Hermann Hall (IIT)



# Map of Lower Level

Hermann Hall (IIT)



## 2010 AIChE Regional Conference: Event Schedule

### Day 1: Thursday, September 30, 2010

	Main Lobby	Herman Lounge	Ballroom	Alumni Lounge	Armour Dining	Trustee Room	Armour Conference	BOG Bar & Stage	Auditorium	Gallery Lounge	Expo Room	Off-site		
7:30am	Registration Table Open	Breakfast										HS Arrive		
8:15am			Welcome & Keynote							HS Welcome and Keynote				
9am														
9:30am														
10am					HS Program	Sustainable Energy Systems	Northwestern Recent Research Results	Design for Sustainability				HS Program	HS Program	
10:30pm														
11pm														
11:30pm														
12pm														
12:30pm														
1pm					HS Program	Process Efficiency Improvements	Renewable Biofuels from Lignocellulose	YPAB Session Innomag Pump Demonstration	YPAB Session - Resume Workshop			HS Program	HS Program	
1:30pm														
2pm														
2:30pm														
3pm														HS Depart
3:30pm						Integrated Renewable Systems for a Green Economy	Renewable Biofuels from Lignocellulose Recent Advances II	Petroleum Refining	YPAB Session - To FE or Not to FE					
4pm														
4:30pm														
5pm														
5:30pm					Buffett Dinner						Poster Session			
6pm														
7pm														
7:30pm -9:00pm								YBAB Entertainment Comedy Night at theBOG						

## 2010 AIChE Regional Conference: Event Schedule

### Day 2: Friday October 1, 2010

	Main Lobby	Herman Lounge	Ballroom	Alumni Lounge	Armour Dining	Trustee Room	Armour Conference	Auditorium	Gallery Lounge	Expo Room	Off-site	
7:30am	Registration Table Open	Breakfast									HS Arrive	
8:15am												
9am			Keynote						HS Welcome and Keynote			
9:30am												
10am			YPAB Improvisation for Engineering Innovation	Process Safety Developments	Energy and the Environment	Perfect Power Implementation, Education, and Research at IIT				HS Program	HS Program	
10:30pm												
11pm												
11:30pm												
12pm												
12:30pm												
1pm												
1:30pm					HS Program	Process Industry Practices	Modeling, Supervision and Control of Processes	Renewable Energy	YPAB Session - Mock Interviews		HS Program	HS Program
2pm												
2:30pm											HS Depart	
3pm												
3:30pm												
4pm - 8:30pm											YPAB Networking Mixer Grace O'Malleys	

## Program Grid: Special Events

Time	Description	Location
<b>Thursday</b> 8:15 - 9:30AM	<b>Thursday Keynote Address</b>	Ballroom
	<b>Illinois Coal 101</b> <b>Bill Hoback</b> , Office of Coal Development, Springfield, IL	
<b>Thursday &amp; Friday</b> 9:15 AM - 1:00PM	<b>High School &amp; Community Outreach Program</b> (see page 20 for more information)	Auditorium
<b>Thursday</b> 5:00 – 7:30 PM	<b>Poster Session and Buffet Dinner</b>	Expo Room
	Come see the latest contributions on topics of interest in chemical engineering research and development. In addition, to networking with chemical engineering peers over dinner.	
<b>Friday</b> 8:15 - 9:30AM	<b>Friday Keynote Address</b>	Ballroom
	<b>Sustainability and the Case for Transformational Research</b> <b>Maria K. Burka</b> , National Science Foundation, Arlington, VA	

## Program Grid: Young Professional Advisory Board Sessions / Events

Time	Description	Location
<b>Thursday</b> 12:30 - 2:30 PM	<b>YPAB Session - Resume Workshop</b> Freshen up your résumé with one-on-one help from local Young Professionals. Make sure to bring your résumé!	Armour Conference
<b>Thursday</b> 3:00 - 5:00PM	<b>YPAB Session - 'To FE or not to FE'</b> Come meet our panel of active Chemical Engineer Professional Engineers and hear first-hand why you need it and what it takes. Impending changes to licensure requirements will also be discussed.	Armour Conference
<b>Thursday</b> 12:30 – 1:30 PM	<b>YPAB Session – INNOMAG Pump Demonstration</b> Professional Matthew Moy from INNOMAG in Addison, IL will lead an interactive demonstration on sealless non-metallic magnetically driven pumps.	Trustee Room
<b>Thursday</b> 7:30 - 9:00 PM	<b>YPAB Event - Comedy Night at the BOG</b> Chemical & Biomolecular Engineering Professor by day, stand-up comedian by night, and host of “Inside the Black Box” on WREK-Radio, Pete Ludovice is out to prove that engineers can be funny and not just funny-looking.	The Bog in Herman Hall at IIT
<b>Friday</b> 9:30 AM - 12:00 PM	<b>YPAB Session – Improvisation for Engineering Innovation</b> This session looks at the approach of using improvisational humor exercises to generate innovative ideas and improve creativity that has traditionally not been used in technical innovation.	Ballroom
<b>Friday</b> 1:00 - 3:30 PM	<b>YPAB Session – Mock Interviews</b> Come practice your interview skills with local Young Professionals and learn tips and tricks to help you land that perfect position.	Armour Conference
<b>Friday</b> 4:00 - 7:00 PM	<b>YPAB Event - Networking</b> Come, relax, and join us for Happy Hour at Grace O'Malleys with drink specials and lively conversation. Soft drinks and appetizers courtesy of YPAB-Chicago.	Grace O'Malleys, 1416 S. Michigan Ave, Chicago, IL

## Program Grid: Technical Sessions - Thursday, September 30, 2010

<b>Welcoming Remarks and Keynote Presentation</b>		<b>Location: Ballroom</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
8:15 - 8:20 AM	Welcoming Remarks	Steve Rosenblum, UOP LLC and Chair of Chicago Section AIChE
8:20 - 9:30 AM	Keynote – Illinois Coal 101	Bill Hoback, Office of Coal Development, Springfield, IL

<b>Sustainable Energy Systems</b>		<b>Location: Alumni Lounge</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
9:30 - 9:55 AM	Renewable Sources in Flexible Fuel Energy Conversion Networks	Jeffrey Kantor and Patrick Mousaw
10:00 – 10:25 AM	Market Responsive Control: A Second Order Approach to Economic Based Controller Design	Benjamin P. Omell and Donald J. Chmielewski
10:30 - 10:55 AM	A System-Level Approach to Advanced Transportation Fuel Production and Use	Mark Petri
11:00 – 11:30 AM	Optimal Sensor Placement for IGCC Power Systems	Adrian J. Lee and Urmila Diwekar

## Program Grid: Technical Sessions - Thursday, September 30, 2010

<b>Design for Sustainability</b>		<b>Location: Trustee Room</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
9:30 – 9:55 AM	Life Cycle Assessments	David Dixon
10:00 – 10:25 AM	Treatment of Industrial, Point Source Waste Streams Using Membrane Filtration Technology	Mike Grigus and Bruce Blanchard
10:30 – 10:55 AM	Sustainability Drivers	Anne Giesecke
11:00 – 11:30 AM	Benchmarks and Roadmaps for Sustainability	Darlene Schuster

## Program Grid: Technical Sessions - Thursday, September 30, 2010

<b>Northwestern Recent Research Results</b>		<b>Location: Armour Dining</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
9:30 - 9:50 AM	Novel Hybrids of Poly(lactic acid) with Microcrystalline Cellulose and Polyethylene Glycol: Major Enhancements In Crystallization Kinetics Leading to Mechanical Robustness near 100 °C	Philip Brunner, John R. Dorgan and John M. Torkelson
9:50 - 10:10 AM	Evaluation of Metal Sites within Metal-Organic Frameworks for Hydroperoxide Decomposition Activity	Patrick Ryan, Linda J. Broadbelt and Randall Q. Snurr
10:10 - 10:30 AM	Synthesis and Understanding of Novel Supported Catalysts for Sustainable Chemicals and Fuels	Justin M. Notestein
10:30 - 10:50 AM	Design of Biomimetic Catalysts Using Molecular Modeling	Ivan A. Konstantinov and Linda J. Broadbelt
10:50 - 11:10 AM	Silicon-Graphene Composites for Li Ion Battery Anodes	Cary M. Hayner, Jung Kyoo Lee, Kurt B. Smith and Harold H. Kung
11:10 - 11:30 AM	Structural Heterogeneity of Lithifying Biofilms In Urinary Catheters	Jisun Lee, Mohanned El-Natour, Daoping Peng, Jennifer Drummond, David Stickler, Denis Keane, Jean-François Gaillard and Aaron Packman

## Program Grid: Technical Sessions - Thursday, September 30, 2010

<b>Renewable Biofuels From Lignocellulose – Recent Advances I</b>		<b>Location: Armour Dining</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
12:30 - 12:55 PM	Global Potential of Rice Hull as a Renewable Feedstock for Fuel Ethanol Production	Badal C. Saha and Michael A. Cotta
1:00 - 1:25 PM	On-Farm Preservation and Pretreatment of Perennial Grasses for Fuel Ethanol Production	Matthew F. Digman, Kevin Shinnors, Michael D. Casler, Bruce S. Dien, Ronald Hatfield, Han-Joachim G. Jung, Richard E. Muck and Paul J. Weimer
1:30 - 1:55 PM	Use of a Microbe to Mitigate Inhibitors in Biomass Fermentations	Nancy N. Nichols, Bruce S. Dien, Badal C. Saha and Michael A. Cotta
2:00 – 2:30 PM	Protein Engineering of GRE2 From <i>Saccharomyces Cerevisiae</i> for Enhanced Detoxification of 5-Hydroxymethyl Furfural	Jaewoong Moon and Z. Lewis Liu

## Program Grid: Technical Sessions - Thursday, September 30, 2010

Process Efficiency Improvements		Location: Alumni Lounge
Time	Presentation Title	Speaker(s)
12:30 – 12:55 PM	An Efficient Stochastic Optimization Framework for Studying the Impact of Seasonal Variation On the Minimum Water Consumption of Pulverized Coal (PC) Power Plants	Juan M. Salazar and Urmila Diwekar
12:50 – 1:10 PM	Process Efficiency for Regeneration of Ammonia Borane	Thanh Hua
1:10 -1:30 PM	Structural Characterization and Theoretical Calculation of Furfuryl Alcohol and Hydroxymethylfurfural	Taejin Kim, Rajeev Assary, Larry Curtis, Christopher Marshall and Peter Stair
1:30-1:50 PM	Pressurized Steam Reforming of Bio-Derived Fuels for Distributed Hydrogen Production – A Systems Model Analysis to Compare System Efficiency	Dionissios D. Papadias, Sheldon Lee and Shabbir Ahmed
1:50 -2:10 PM	Compact Heat Exchange Reactor In Fischer-Tropsch Process Application	Zhijun Jia and Larry Stryker
2:10 – 2:30 PM	Vibrational Properties of Levulinic Acid and Furan Derivatives: Raman Spectroscopic and Theoretical Calculation	Taejin Kim, Rajeev Assary, Larry A. Curtiss, Christopher L. Marshall and Peter C. Stair

## Program Grid: Technical Sessions - Thursday, September 30, 2010

<b>Renewable Biofuels From Lignocellulose – Recent Advances II</b>		<b>Location: Armour Dining</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
3:00 – 3:25 PM	Reprogrammed Glucose Metabolic Pathways of Inhibitor-Tolerant Yeast	Z. Lewis Liu, Menggen Ma and Michael A. Cotta
3:30 – 3:55 PM	Process Design Considerations for Optimal Production of Ethanol From Lignocellulose Using Available Yeasts, Including Natural Pentose-Fermenting Yeasts, and Their Derivatives	Patricia J. Slininger, Jaewoong Moon and Z. Lewis Liu
4:00 – 4:25 PM	Novel Developments in Butanol Fermentation: Microbial Genetics to Agricultural Substrates, Process Technology, and Downstream Processing	Nasib Qureshi, Siqing Liu, Badal C. Saha and Michael A. Cotta
4:30 – 4:55 PM	Optimal Control of Biodiesel Production In a Batch Reactor In the Face of Feed Variability	Pahola T. Benavides and Urmila Diwekar

<b>Petroleum Refining – Factoring in Reliability</b>		<b>Location: Trustee Room</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
3:00 - 3:25 PM	High Acid Crude Processing: Corrosion Control Strategies	Randy Rechten
3:30 - 3:50 PM	Risk Management of High Temperature Refinery Equipment	Peter Carter, Chris Matice and Claudio Allevato
4:00 – 4:30 PM	Reliability Planning & Execution In Refining Projects	Tom Brindley and Mike Hammond

## Program Grid: Technical Sessions - Thursday, September 30, 2010

<b>Integrated Renewable Systems for a Green (\$) Economy</b>		<b>Location: Alumni Lounge</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
3:00 - 3:25 PM	Clean and Renewable Energy Policy and Program Recommendations	Suzanne Malec-McKenna and Howard Learner
3:30 - 3:50 PM	The Carbon and Energy Footprint of Water Treatment, Distribution and Reclamation and Waterway Management In Greater Chicago	Pete Mulvaney, Catherine A. O'Connor, Antonio Quintanilla, Louis Kollias, Manju Sharma and Richard Lanyon
4:00 - 4:25 PM	The Emerald Forest– Algae Production In a Pilot-Scale Photobioreactor	Fouad Teymour
4:30 - 5:00 PM	Heat Recovery at a Water Reclamation Plant In Greater Chicago	Ali K. Oskouie, Catherine A. O'Connor, David Lordi, Louis Kollias and Richard Lanyon

## Program Grid: Technical Sessions - Friday, October 1, 2010

<b>Keynote Presentation</b>		<b>Location: Ballroom</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
8:15 - 9:30 AM	Keynote – Engineering Programs and Initiatives at the National Science Foundation	<b>Maria K. Burka</b> , National Science Foundation, Arlington, VA

<b>Perfect Power Implementation, Education, and Research at IIT</b>		<b>Location: Trustee Room</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
9:30 – 9:55 AM	Perfect Power Implementation at Illinois Institute of Technology	Joseph Clair
10:00 – 10:25 AM	Autonomous Agents for Advanced Distribution Automation In Perfect Power Systems	Alex Flueck
10:30 – 10:55 AM	Update on IIT Microgrid Master Controller	Greg Rouse
11:00 – 11:25 AM	Application of Zigbee Wireless In Smart Grid	Chi Zhou
11:30 – 11:55 AM	Illinois Institute of Technology Smart Grid Education and Workforce Training Center	Melissa Gordon

## Program Grid: Technical Sessions - Friday, October 1, 2010

<b>Process Safety Developments</b>		<b>Location: Alumni Lounge</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
9:30 - 9:55 AM	Materials Signature of Fires	Robert O'Shea Jr.
10:00 - 10:25 AM	Safety Critical Instrumentation Testing Guidelines	Peter G. Herena and Yasser Ali Khalil
10:30 – 10:55 AM	Guide to Developing and Implementing Safety Checklists: Plant Steam Utilities	Juan C. Ramirez, Mark Fecke, John Martens and Delmar R. Morrison
11:00 – 11:30 AM	Considerations for Relief System Design of Reactive Chemical Systems	Amy Theis

## Program Grid: Technical Sessions - Friday, October 1, 2010

<b>Energy and the Environment</b>		<b>Location: Armour Dining</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
9:30 - 9:55 AM	Study of Absorption Based Carbon Capture In a Coal Fired Power Plant	Prakash Kotecha and Urmila Diwekar
10:00 - 10:25 AM	Characterization and Stochastic Modeling of Uncertainties In the Biodiesel Production	Urmila Diwekar and Sheraz Abbasi
10:30 – 10:55 AM	Potential Impacts of PHEVs on Regional Power Systems	Jianhui Wang and Cong Liu
11:00 – 11:25 AM	An Overview of the Energy-Water Nexus	Leslie Poch
11:30 – 11:55 AM	Collaboration and Technology Usher In the Era of Shale Gas	Trevor Smith

<b>Process Industry Practices</b>		<b>Location: Alumni Lounge</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
1:00 – 1:25 PM	A Breakthrough In Flue Gas Cleanup, CO2 Mitigation and H2S Removal	Wolf Koch
1:30 – 2:00 PM	Beryllium and Modern Day Alchemy	Paul Jahn

## Program Grid: Technical Sessions - Friday, October 1, 2010

<b>Modeling, Supervision and Control of Chemical, Biological and Pharmaceutical Processes</b>		<b>Location: Armour Dining</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
1:00 – 1:25 PM	Control of Complex Systems with Applications to Polymerization Reactors	Fouad Teymour
1:30 – 1:55 PM	Integrating Design and Control by Embedded Control Optimization Method	Andreas A. Linninger
2:00 – 2:25 PM	Modeling of Biochemical Reactors – Role In Analysis, Design, Optimization and Control	Satish J. Parulekar
2:30 – 2:55 PM	New Trends In Monitoring and Supervision of Distributed Processes: Towards Fault-Tolerant Control	Ali Cinar
3:00 – 3:25 PM	Industrial Applications of Rule-Based Systems	Jeffrey D. DeCicco

## Program Grid: Technical Sessions - Friday, October 1, 2010

<b>Renewable Energy</b>		<b>Location: Trustee Room</b>
<b>Time</b>	<b>Presentation Title</b>	<b>Speaker(s)</b>
1:00 – 1:25 PM	Biofuels and BioEnergy Overview	Stanley Frey
1:25 – 1:50 PM	Pennycress: a Sustainable Energy Crop for Biofuels Production	Peter B. Johnsen
1:50 – 2:15 PM	Syngas to Ethanol	Steve Donnellan
2:15 – 2:40	Integrated Bio-Refinery Automation Solutions	Ganesh Venimadhavan



The American Institute of Chemical  
Engineers  
And The University of Illinois Chicago  
WELCOMES MIDDLE & HIGH SCHOOL  
STUDENTS  
September 30<sup>th</sup> and October 1st, 2010



## High School Outreach Program

### Being an Engineer—Creating A World That Works!

- 9:15 – 9:30 AM**      **Welcome and Opening Comments**  
Alan Zagoria, Chemical Engineer, UOP
- 9:30 – 10:00 AM**    **Introduction to Engineering**
- 10:00 – 11:00 AM**   **Chemical Engineering in Space**  
Albert Sacco Jr., Ph.D., ex-NASA Astronaut, Chemical Engineering Professor  
Professor Sacco received a B.S. in Chemical Engineering from Northeastern University in 1973 and a doctorate from the Massachusetts Institute of Technology. He rose to the position of head of the Department of Chemical Engineering at Worcester Polytechnic Institute before returning to Northeastern as professor and Director of the NASA-sponsored Center for Advanced Microgravity Materials Processing. He flew on the space shuttle Columbia in 1995 as a payload specialist, conducting over 200 experiments for many scientists in an environment with approximately one millionth of the earth's gravity.
- 11:00 – 11:45 AM**   **The Engineering Experience: A Panel Discussion**
- 11:45 – 12:00 PM**   **What Kind of Engineer am I?**  
Emceed by Alan Zagoria, Chemical Engineer, UOP  
Participants: Selected Student Representatives
- 12:00 - 1:00 PM**    **Lunch & Chat with Professional Engineers**  
A time for personal conversation with real engineers  
Hosted by UIC and the AIChE Chicago Section
- 1:00 – 1:30 PM**      **Lab Tours**
- 1:30 - ?**              **Co-gen Plant Tour**

# Keynote Address - Thursday

## *Illinois Coal 101*

Thursday, September 30, 2010: 8:15 – 9:30 AM

Ballroom (Illinois Institute of Technology)

**Bill Hoback**, Office of Coal Development, Springfield, IL

Mission: DCEO's Office of Coal Development is dedicated to the development and use of Illinois' extensive coal resources as a fuel source for the 21st Century. Coal not only plays a vital role as an energy source, but the industries involved in the mining, transportation and use of coal provide billions of dollars in economic activity, thousands of jobs for Illinoisans and stability to many communities across the state.

Vision: The Office of Coal Development seeks to advance carbon capture and storage technologies; provide financial incentives for advanced gasification projects using Illinois coal; develop and promote new markets for Illinois mined coal and coal byproducts; and promote a comprehensive, long-range energy policy that secures America's energy future and creates jobs.

Gone are the pick axes, mules, wooden carts and canaries in a cage. Today's underground mines use highly-mechanized equipment to cut and transport coal. Sophisticated technology monitors the atmosphere and controls coal dust in the work environment. Surface mines bustle in well-choreographed motion that increases mining efficiency and productivity. In all cases, the surface land is restored to previous productivity standards after the coal is extracted. All of this is done while protecting the health of the workers and the environment.

The Illinois Basin covers nearly 37,000 square miles in Illinois and in portions of Indiana and western Kentucky. Coal deposits began to form more than 300 million years ago during the Pennsylvanian Period, when the land that is now Illinois was near the Equator. Thick mats of plant debris accumulated on the floor of tropical swamps and were buried to form peat. Over millions of years, the layers of peat were compressed into coal. This process created more than 75 layers or "seams" of coal that range from a few inches up to ten-feet thick. Some of the coal seams cover thousands of square miles in Illinois and adjacent states, but most occur in small, more limited areas.

Illinois continues to be well-positioned for any demand-led rebound for its still-underdeveloped coal resources. Certain new market growth is anticipated as coal from the Illinois Basin displaces Appalachian coal, based on price spread, as well as in markets where new power plant air emissions controls remove decades-long advantages for lower-sulfur fuels. Growth also hinges on how export markets evolve and how uncertainties are resolved regarding federal CO<sub>2</sub> cap-and-trade law, or other new environmental regulations. Selection as host site for the \$2 billion, near-zero-emissions FutureGen project attests to the position of national leadership Illinois has established in the field of carbon capture and sequestration. It is the capstone of an effort, led by the Office of Coal Development, in which Illinois has pursued a public policy of fostering deployment of coal gasification facilities that are the needed linkage to the future of coal in what is likely to be a carbon-constrained world.

Current research promises to reduce coal's carbon footprint. The Office of Coal Development is working to make coal a clean bridge to a bright future.

#### Biography:

Bill Hoback, is in his eighth year leading the nation's most aggressive and broad-based state program aimed at stimulating coal utilization through initiatives in deploying clean coal technology at The Office of Coal Development. Hoback took over coal development at the Department of Commerce and Economic Opportunity after serving for several years as Illinois Coal Industry Liaison for the United Mine Workers of America, District 12. His responsibilities included coal education programs, government relations, and employment and training issues. He first went to work for the UMWA in 1996 in the union's Washington D.C. legislative office. Hoback, as coordinator of the Illinois FutureGen effort, put together a winning team of scientists, engineers, educators, state and local elected officials and economic development professionals. The team worked intensely for over two years on the world-class, near-zero emissions FutureGen project. Mattoon, Illinois was chosen in December 2007 as the FutureGen site. Hoback also has led state efforts to foster development of the 1,600-megawatt Prairie State Energy Campus in southwestern Illinois. In addition, he has helped reach the Taylorville Energy Center ground-breaking stage, where 735 megawatts of electricity will be produced, along with pipeline quality synthetic natural gas (SNG). Another major accomplishment has been Illinois' adoption of the nation's first Clean Coal Portfolio Standard, giving coal-fueled, carbon capture technology electric plants access to the state's de-regulated power market.

## **Keynote Address - Friday**

### ***Engineering Programs and Initiatives at the National Science Foundation***

Friday, October 1, 2010: 8:15 – 9:30 AM

Ballroom (Illinois Institute of Technology)

**Maria K. Burka**, National Science Foundation, Arlington, VA

Recent emphases at the National Science Foundation include Cyber-enabled Discovery and Innovation (the application of cyberinfrastructure to the various domains such as chemical engineering), energy (development of alternative sources to possibly replace fossil fuels) and the environmental, bioengineering, and complex systems. Details of programs dealing with these topics as well as core chemical engineering programs, including proposed and actual budgets, will be discussed, including their relevance to National Academy of Engineering grand challenges.

#### Biography:

Maria Burka is program director of Process and Reaction Engineering in the Chemical, Bioengineering, Environmental, and Transport Systems Division of the National Science Foundation. She was a process design engineer with Scientific Design Co. (New York, NY), a faculty member at the Univ. of Maryland, College Park, and a Senior Scientist with EPA. Maria received her BS and MS from MIT, and her MA and PhD from Princeton Univ., all in chemical engineering. An AIChE Fellow and 2010 AIChE President-Elect, Maria has served on AIChE's Board of Directors; as Director and Chair of the Catalysis and Reaction Engineering Division; Director and Secretary/Treasurer of the Computing and Systems Technology Division; Chair of the National Capital Section; Meeting Program Co-Chair of the 2003 Annual Meeting; and on the Constitution and By-Laws, Women's Initiatives, and Steering Committees. She heads the Washington Internships for Students of Engineering (WISE) summer program for AIChE, is Vice Chair of the International Committee, and is a member of the Admissions Committee. She is involved in the American Chemical Society, Sigma Xi, the Society of Women Engineers, and the American Association of University Women.

# Sustainable Energy Systems

Thursday, September 30, 2010: 9:30 AM

Alumni Lounge (Illinois Institute of Technology)

## Description:

Energy research includes various areas of research like biomass energy, conventional energy, carbon capture, direct solar fuels, building efficiency, energy storage, renewable power, vehicle technology, waste heat capture, and water. Although, each area can bring in individual components that are optimized for performance, an overarching session is necessary for development and insertion of next generation integrated energy systems. The focus this session will be on the systems view. The system perspective will include renewable energy systems and resource limited energy systems like fossil fuels. The aim of this session is to present feasible, reliable, flexible, cost effective, efficient and environmentally friendly energy systems.

## Chair:

Urmila Diwekar

Email: [urmila@vri-custom.org](mailto:urmila@vri-custom.org)

## *Renewable Sources In Flexible Fuel Energy Conversion Networks*

Thursday, September 30, 2010: 9:30 AM

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Jeffrey Kantor, Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN and  
Patrick Mousaw, Department of Chemical & Biomolecular Engineering, University of Notre Dame, Notre  
Dame, IN

Using principles from finite-time thermodynamics, we demonstrate a novel class of bilinear models suitable for the modeling of flexible energy conversion networks appropriate for use in campus scale and municipal scale utilities with complex energy requirements, fuel sources, and operational flexibility. A previous report focused on the use of the bilinear models for estimating the efficiency of complex and flexible energy conversion networks [2]. Financially optimal operating conditions and opportunities for financial and operational hedging may be determined from these models [1, 3]. We incorporate renewable sources of energy conversion into the energy conversion network modeling. These renewable sources are modeled using the same components and techniques used in modeling traditional fossil fuel-based plants. We demonstrate multi-engine and cogeneration energy conversion network models utilizing a combination of fossil fuel-based and renewable energy sources. Valuation of the flexibility to use renewable sources to generate energy is computed. This is demonstrated with several examples. In summary, we present the following main results: \* Modeling of flexible fossil fuel and renewable energy source energy conversion networks is demonstrated, \* Valuation of the flexibility introduced by including renewable sources is calculated for several examples.

## *Market Responsive Control: A Second Order Approach to Economic Based Controller Design*

Thursday, September 30, 2010: 10:00 AM

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Benjamin P. Omell and Donald J. Chmielewski, Chemical and Biological Engineering, Illinois Institute of  
Technology, Chicago, IL

The economics of plant operations are greatly influenced by the cost of utilities. While the price of fuel is typically a slowly varying parameter, the cost of electricity tends to change quickly. While classic control schemes have no ability to respond to utility costs, advance controllers typically are capable, but only through the Real-Time Optimization (RTO) algorithm, which takes a steady-state perspective on the cost of

utilities. Thus, in the case of electricity price variations, which have a time scale on the order of most chemical processes, an RTO approach will be insufficient to capture the fast changes associated with electricity markets. The notion of Market Responsive Control aims to exploit measurements and the fairly regular cycle of electricity price to achieve a maximum in average profit (by defraying energy intensive operations until prices are low). The effort focuses on the design of a high level (supervisory) control system that is capable of market responsiveness. That is, design a controller that uses the electricity spot price as a disturbance input to the decision making process. However, in contrast to traditional controller designs, where the objective is to attenuate disturbances, the Market Responsive Controller will judiciously amplify the spot price disturbance. We have found that a Linear Quadratic Gaussian controller can be forced to have such behavior if the cross-term weights of the objective function are utilized. However, it is a non-trivial task to select weights such that profit is maximized, while observing the equipment limitations. Thus, the core result of the paper is the development of a profit maximizing scheme for the selection of LQG weights subject to process equipment limitations. The resulting optimization problem will be shown to be convex and thus will yield a globally optimal solution. The methodology will be illustrated by application to an Integrated Gasification Combined Cycle (IGCC) as well as a building HVAC system. If time permits, a globally optimal scheme for the sizing and selection of energy storage units will also be presented.

## *A System-Level Approach to Advanced Transportation Fuel Production and Use*

**Thursday, September 30, 2010: 10:30 AM**

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Mark Petri, Energy Engineering and System Analysis, Argonne National Laboratory, Chicago, IL

World energy demand is expected to increase thirty-six percent by 2030, much of which will be in the form of petroleum-based liquids for transportation. The need for fossil fuels for transportation in the U.S. will likewise continue to grow. The result is that, despite efforts to reduce greenhouse gas emissions, carbon dioxide emissions in the U.S. are expected to grow by seven percent by 2030.

The development of alternative transportation fuels that do not rely on petroleum and that have smaller life-cycle carbon costs have been a major focus of federal research efforts. Many of the proposed alternative fuels are not yet cost effective because of the limits of existing materials, chemicals, devices, and processes. Argonne is taking an integrated approach that focuses on critical pathways necessary for the large-scale deployment of advanced transportation fuels. The laboratory is pursuing photo/electro-chemical, photo-biological, and thermal catalytic routes to new liquid fuels, integrated with holistic engine design and optimization. Argonne is taking a system-level approach to research on new feedstock, processing, combustion science, modeling, real-world testing, optimization, and life-cycle analysis.

Examples of this work include significant discoveries in engineering photosynthetic bacteria for long-chain biofuel precursor production, improving the efficiency of product separation, and in identifying and modeling key reactions for fuel ignition at elevated pressure.

## *Optimal Sensor Placement for IGCC Power Systems*

**Thursday, September 30, 2010: 11:00 AM**

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Adrian J. Lee, Vishwamitra Research Institute, Clarendon Hills, IL and Urmila Diwekar, Vishwamitra Research Institute, Center for Uncertain Systems: Tools for Optimization and Management, Clarendon Hills, IL

The optimal sensor placement problem involves determining the most effective locations to place a network of sensors across an array of measurable signals, in accordance with a set of specified objectives and constraints, such as cost, performance, and sensitivity to variations in uncertain environments. In advanced power systems, such as in Pulverized Coal (PC) and Integrated Gasification Combined Cycle (IGCC) power plants, the placement of sensors on-line within the power generation process can be expensive or technically infeasible due to certain harsh environments. This paper uses advanced modeling techniques to simulate the system's behavior to variability in process variables. This variability is analyzed using a technique from information theory to determine the most cost-effective network of on-line sensors by formulating a nonlinear, stochastic binary integer problem. The solution is achieved by using an efficient sampling technique, Better Optimization algorithm for Nonlinear Uncertain Systems (BONUS). The key contribution of using Fisher information as a metric for observability is that it generalizes the Gaussian assumption on representing process and measurement variability for systems governed by nonlinear dynamics.

# Design for Sustainability

**Thursday, September 30, 2010: 9:30 AM**  
Trustee Room (Illinois Institute of Technology)

## **Description:**

Sustainability, especially in facility design and construction can have many meanings. The food industry has been among the leaders in manufacturing to apply LEED principles to building designs and expansions. LEED stands for Leadership in Energy and Environmental Design, and is a program managed by the USGBC, U.S. Green Building Council. Speakers in this session will present cases of success and discuss future opportunities for good chemical engineering applications to energy conservation, recycling and reuse.

## **Chair:**

J. Peter Clark  
**Email:** [jpc3@att.net](mailto:jpc3@att.net)

## **Co-Chair:**

David Dixon  
**Email:** [ddixon@burnsmcd.com](mailto:ddixon@burnsmcd.com)

## *Life Cycle Assessments*

**Thursday, September 30, 2010: 9:30 AM**  
[Trustee Room \(Illinois Institute of Technology\)](#)  
David Dixon, Food and Consumer Products, Burns & McDonnell, Alpharetta, GA

Life Cycle Assessments are used to quantify the impacts to our environment of alternate food processes. In the broadest reach of the assessment technique, the analysis encompasses from “farm to fork”. This is a developing technique intended to guide decision makers that need to understand more fully the impact to greenhouse gases, land use, ozone depletion, acidification of water bodies or soils, smog, nutrient overload of surface waters, or other impacts that are considered relevant. LCA can be used in product design, supply chain decisions, marketing, negotiations with suppliers, etc with a goal to providing a more sustainable product to customers. This can a complex and difficult method, but needs to be better understood by those considering its use or being asked by customers to do these calculations. This presentation will survey the use of LCA in the US and abroad, giving examples of decisions made based on the results of a life cycle assessment.

## *Treatment of Industrial, Point Source Waste Streams Using Membrane Filtration Technology*

**Thursday, September 30, 2010: 10:00 AM**  
[Trustee Room \(Illinois Institute of Technology\)](#)  
Mike Grigus, Liquid Processing Division, GEA Process Engineering Inc., Hudson, WI and Bruce Blanchard, GEA Process Engineering Inc., Hudson, WI

The presentation will provide an overview on the use of microfiltration (MF), ultrafiltration (UF), nanofiltration (NF), and reverse osmosis (RO) membrane technology in the treatment of industrial, point source waste streams for the dairy, food, beverage, biotech, and chemical industries. In addition, specific applications and their solutions will be explained with information provided on operating, performance, and cost parameters.

## *Sustainability Drivers*

**Thursday, September 30, 2010: 10:30 AM**

Trustee Room (Illinois Institute of Technology)

Anne Giesecke, A & D Policy Analysis, Inc., Lincoln, NE

Sustainability is being driven by accountability. Companies are being held accountable by retail customers and consumers, stock holders, insurance companies, and governments. The food industry has responded with operating efficiencies while maintaining safety and quality.

## *Benchmarks and Roadmaps for Sustainability*

**Thursday, September 30, 2010: 11:00 AM**

Trustee Room (Illinois Institute of Technology)

Darlene Schuster, AIChE, New York, NY

Sustainability can be approached and measured from many levels—corporate, process, product and individual professionals. An overview will be presented of various ways to benchmark and measure sustainability at these levels and major initiatives of the AIChE Institute for Sustainability will be highlighted. The AIChE Sustainability Index (sm) and the Center for Sustainable Technology Practices Sustainability Framework, and efforts to develop a certification program for individual practitioners of sustainability will be reviewed. The roles of benchmarking sustainability performance and the utility of such benchmarks for the chemical industry as they approach greening along their supply chains will also be discussed.

## Northwestern Recent Research Results

Thursday, September 30, 2010: 9:30 AM  
Armour Dining (Illinois Institute of Technology)

### Description:

This session will discuss cutting edge research in the department of chemical and biological engineering at Northwestern University. This research emphasizes the design and understanding of new materials and processes for sustainability. The areas of transport phenomena, electrical storage materials, polymer processing, separations materials, and catalysis are highlighted.

### Chair:

Justin M. Notestein

Email: [j-notestein@northwestern.edu](mailto:j-notestein@northwestern.edu)

### *Novel Hybrids of Poly(lactic acid) with Microcrystalline Cellulose and Polyethylene Glycol: Major Enhancements In Crystallization Kinetics Leading to Mechanical Robustness near 100 °C*

Thursday, September 30, 2010: 9:30 AM

Armour Dining (Illinois Institute of Technology)

Philip Brunner, Materials Science and, Northwestern University, Evanston, IL, John R. Dorgan, Chemical Engineering, Colorado School of Mines, Golden, CO and John M. Torkelson, Chemical and Biological Engineering and Materials Science & Engineering, Northwestern University, Evanston, IL

Overcoming the technological challenges associated with low melt-state thermal stability, grudgingly slow crystallization, and low heat distortion temperature is essential for the full commercial potential of poly(lactic acid) (PLA) to be realized. We address this challenge by preparing PLA composites with low levels of biobased microcrystalline cellulose (MCC) via a continuous, industrially scalable process called solid-state shear pulverization (SSSP), which exposes polymers to high shear and compressive forces near ambient temperature. We can then follow this with melt processing (MP) with added polyethylene glycol (PEG). Differential scanning calorimetry reveals that upon cooling at 60 °C/min from the melt state, an 89/1/10 wt% PLA/MCC/PEG composite made by SSSP/MP exhibits 30% PLA crystallinity, compared with < 1% crystallinity for both as-received PLA pellet and 99/1 wt% PLA/MCC composite and near the 40-45% maximum PLA crystallinity obtained after long-time isothermal crystallization. Relative to neat, unprocessed PLA, an 89/1/10 wt% PLA/MCC/PEG hybrid made by SSSP/MP also exhibits a factor of 30 reduction in isothermal (105 °C) crystallization half-time, whereas the 99/1 wt% PLA/MCC composite demonstrates a factor of 20 reduction. Dynamic mechanical analysis reveals that the 89/1/10 wt% PLA/MCC/PEG hybrid requires only 30 sec annealing at 105 °C in a hot press to develop sufficient crystallinity to prevent distortion at temperatures far above PLA's glass transition temperature (60 °C); in contrast, a 99/1 wt% PLA/MCC blend and neat PLA require over 3 and 10 min of annealing, respectively. The 30 sec annealing step is within standard injection molding cycles and significantly broadens possible applications of PLA. This study demonstrates that SSSP with biodegradable fillers may provide a green solution to the challenges associated with PLA and that sustainable engineering of polymers can be synonymous with property improvement.

## *Evaluation of Metal Sites within Metal-Organic Frameworks for Hydroperoxide Decomposition Activity*

**Thursday, September 30, 2010: 9:50 AM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Patrick Ryan<sup>1</sup>, Linda J. Broadbelt<sup>2</sup> and Randall Q. Snurr<sup>2</sup>, (1)Chemical & Biological Engineering, Northwestern University, Evanston, IL, (2)Chemical and Biological Engineering, Northwestern University, Evanston, IL

Autooxidation is an important industrial process for converting raw hydrocarbon materials to more useful oxidized products. Recently, Corma and coworkers (Xamena et al., J. Catal., 2008, 255, 220) showed that cobalt- and copper-containing MOFs were active for peroxide decomposition during tetralin autooxidation. Using density functional theory (DFT), we studied decomposition reactions over different metal clusters that are representative of the repeating metal sites in each MOF. Our DFT results suggest that the tetrahedral cobalt site in Co-MOF is too sterically protected to catalyze hydroperoxide decomposition. Additionally, carboxyl groups of the linkers in Cu-MOF seem to shield the copper sites from hydroperoxide species and hinder catalysis. For these two cases, we believe catalysis observed by Xamena et al. likely occurs on the outer surface of the MOF crystals. We have mapped a possible decomposition pathway of hydroperoxide molecules over a copper paddlewheel, which is found both in the HKUST-1 material and the series of NOTT materials. Our results suggest that catalysis appears to be possible over copper paddlewheels in MOFs, and this work may lead to new, improved oxidation catalysts in the future.

## *Synthesis and Understanding of Novel Supported Catalysts for Sustainable Chemicals and Fuels*

**Thursday, September 30, 2010: 10:10 AM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Justin M. Notestein, Chemical and Biological Engineering, Northwestern University, Evanston, IL

This talk will describe recent work in the Notestein laboratory on developing new routes to supported oxide catalysts. Recent efforts have focused on synthesizing highly dispersed Ti, Ta, and Fe oxides on SiO<sub>2</sub> using bulky inorganic complexes as precursors. Highly multidentate organic ligands are chosen such that isolation is maintained in the immobilized species, leading to improved rates and selectivities in alkane oxidation (adamantane to adamantanol with hydrogen peroxide, test reaction), hydroamination, or epoxidation with hydrogen peroxide and organic hydroperoxides. By a slightly different route, supported Mn oxides form cooperative surface catalysts with grafted carboxylic acids, leading to exceptional productivity in epoxidation/dihydroxylation. Finally, glucose isomerization for biomass conversion has been studied over many of these same catalysts.

## *Design of Biomimetic Catalysts Using Molecular Modeling*

**Thursday, September 30, 2010: 10:30 AM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Ivan A. Konstantinov and Linda J. Broadbelt, Chemical and Biological Engineering, Northwestern University, Evanston, IL

Over the course of millions of years nature has perfected the art of catalysis to an extent that only recently researchers are beginning to fully understand and emulate. The efficiency with which enzymes promote biologically relevant reactions has been known for a few decades but only in the past several years species that utilize similar catalytic mechanisms have been investigated. In order to apply the principles of enzymatic catalysis, organic and bio-inorganic chemistry has focused on the search for structural and functional enzymatic models. In this talk, we present our latest research which employed molecular modeling to understand the structure and origins of cooperative interactions in a series of biomimetic organic and bio-inorganic catalysts at the atomistic level. As a consequence, we were able to recommend the rational design of bionic catalysts with high performance.

## *Silicon-Graphene Composites for Li Ion Battery Anodes*

**Thursday, September 30, 2010: 10:50 AM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Cary M. Hayner, Jung Kyoo Lee, Kurt B. Smith and Harold H. Kung, Chemical and Biological Engineering, Northwestern University, Evanston, IL

Rechargeable batteries with large storage capacity and power density have many potential applications in portable electronics, transportation, and load leveling for renewable power sources. Li-ion batteries are the most promising to capitalize on these opportunities, but new materials with much higher energy densities are required for energy-intensive applications. Silicon, with its high gravimetric and volumetric energy density, is an attractive candidate to replace graphite as the anodic material in a Li-ion battery (3579 and 372 mAh/g, respectively). Unfortunately, the intrinsic ~300% volume expansion/contraction during charge-discharge cycling causes silicon particles to fracture, diminishing electrical contact of the particles with other electrode components, resulting in poor cycling performance. Recently, we have developed nanocomposites composed of silicon nanoparticles dispersed between graphene sheets. These freestanding composites are formed by vacuum filtration, and form a highly conductive 3D network of graphene and reconstituted graphite after thermal reduction, thereby minimizing the need for conductive additives and heavy metallic current collector as support. These composites show improved Li-ion storage capacities and cycling stability compared to admixed samples of silicon nanoparticles and carbon support. Whereas silicon nanoparticles mixed with conductive carbon and PVDF binder typically completely degrade within the first 10 cycles, our silicon-graphene composites can achieve initial capacities >2000 mAh/g and maintain capacities over 1200 mAh/g after 100 cycles. Characterization of these composites with various processing and electrochemical conditions will be presented.

## *Structural Heterogeneity of Lithifying Biofilms In Urinary Catheters*

**Thursday, September 30, 2010: 11:10 AM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Jisun Lee<sup>1</sup>, Mohanned El-Natour<sup>2</sup>, Daoping Peng<sup>3</sup>, Jennifer Drummond<sup>1</sup>, David Stickler<sup>4</sup>, Denis Keane<sup>5</sup>, Jean-François Gaillard<sup>3</sup> and Aaron Packman<sup>3</sup>, (1)Chemical and Biological Engineering, Northwestern University, Evanston, IL, (2)Department of Biomedical Engineering Northwestern University, Northwestern University, Evanston, IL, (3)Department of Civil and Environmental Engineering, Northwestern University, Evanston, IL, (4)Cardiff School of Biosciences, Cardiff University, CF10 3AX, United Kingdom, (5)Advanced Photon Source, Argonne National Laboratory, Argonne, IL

The crystalline biofilms formed by *Proteus mirabilis* on Foley catheters can block the flow of urine from the bladder and cause serious complications in the care of many patients undergoing long-term bladder catheterization. We employed a novel approach to investigate the microstructure of catheter encrustations caused by *P. mirabilis*. Synchrotron-based x-ray micro-tomography (XMT) was used to non-invasively acquire high-resolution three-dimensional images of crystalline *P. mirabilis* biofilms in sectioned catheters. These images show that the biofilm structure is highly heterogeneous in terms of both the degree of encrustation and in the porosity and density of the deposits. The detailed, 3D micro-structural information provided by this method supports quantitative analysis of patterns in the crystalline matrix that are important for biofilm development. Unlike conventional biofilms, the crystalline matrix has a (semi)permanent structure that can constrain subsequent biofilm growth. The XMT imaging method presented here provides unique data that is needed to understand these constraints in crystalline biofilms, which occur in a variety of contexts besides urinary tract infections. This method also has great promise for identifying the way in which these crystalline encrustations protect *P. mirabilis* and other urinary pathogens from disinfection and block the efficacy of antimicrobial catheters.

# Renewable Biofuels From Lignocellulose - Recent Advances I

Thursday, September 30, 2010: 12:30 PM  
Armour Dining (Illinois Institute of Technology)

## Description:

The Energy Independence and Security Act of 2007 seeks to expand biofuel production to 36 billion gal/yr by 2022 to replace 20% of our gasoline and targets at least 60% to be advanced biofuels including those produced from lignocellulose. Lignocellulose is an abundant, low-cost, non-food, non-feed feedstock for the production of biofuels. It is available in the form of crop waste matter, such as corn stover, dedicated bioenergy crops, such as switchgrass or Miscanthus, and municipal and forestry wastes. However, significant technical challenges must be overcome to achieve cost-competitive conversion of these feed-stocks. The fibrous cell-wall material that constitutes lignocellulosic feed-stocks is difficult to deconstruct and depolymerize into fermentable sugars. The pretreatment required to open the structure to subsequent enzymatic hydrolysis tends to result in dilute solutions of hexose and pentose sugars containing inhibitors that deter subsequent fermentation to biofuel by microorganisms. Advancements in pretreatments, enzymes and microorganisms to improve resilience, efficiency and cost-effectiveness are emerging. These are being incorporated into processes to be optimized for economical biofuel production from lignocellulose. Progress in this area promises to meet national priorities to reduce dependence on foreign oil, lower greenhouse gas emissions, and promote the rural economy. Presentations will emphasize recent advancements in biocatalytic tools and processes for production of biofuels from lignocellulose.

## Chair:

Patricia J. Slininger

Email: [Pat.Slininger@ars.usda.gov](mailto:Pat.Slininger@ars.usda.gov)

## *Global Potential of Rice Hull as a Renewable Feedstock for Fuel Ethanol Production*

Thursday, September 30, 2010: 12:30 PM  
[Armour Dining \(Illinois Institute of Technology\)](#)

Badal C. Saha and Michael A. Cotta, Bioenergy Research Unit, National Center for Agricultural Utilization Research, USDA-ARS, Peoria, IL

Rice hulls, a complex lignocellulosic material with high lignin (16%) and ash (20%) content, contain about 35% cellulose and 12% hemicellulose and have the potential to serve as a low cost feedstock for production of fuel ethanol globally. Three pretreatment options (dilute acid, lime and alkaline peroxide) and enzymatic saccharification were evaluated for conversion of rice hull cellulose and hemicelluloses to fermentable sugars. The production of ethanol from rice hull hydrolyzate by a mixed sugar utilizing ethanologenic recombinant *Escherichia coli* strain was investigated using both separate hydrolysis and fermentation (SHF) and simultaneous saccharification and fermentation (SSF) approaches. In this presentation, our studies on the conversion of rice hulls to ethanol including recovery of silica will be described. The results show promise in developing an integrated process technology for production of fuel ethanol from rice hulls as a lignocellulosic feedstock.

## *On-Farm Preservation and Pretreatment of Perennial Grasses for Fuel Ethanol Production*

**Thursday, September 30, 2010: 1:00 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Matthew F. Digman<sup>1</sup>, Kevin Shinnars<sup>1</sup>, Michael D. Casler<sup>2</sup>, Bruce S. Dien<sup>3</sup>, Ronald Hatfield<sup>2</sup>, Han-Joachim G. Jung<sup>4</sup>, Richard E. Muck<sup>2</sup> and Paul J. Weimer<sup>2</sup>, (1)Biological Systems Engineering, University of Wisconsin, Madison, WI, (2)U.S. Dairy Forage Research Center, USDA-ARS, Madison, WI, (3)USDA-ARS NCAUR, Peoria, IL, (4)Plant Science Research Unit, USDA-ARS, St. Paul, MN

Recently, wet storage methods have been proposed for feedstock preservation and on-farm storage of perennial grass and corn stover biomass. The advantages over a dry storage system include lower risk of fire, reduced harvest costs, and improved feedstock susceptibility to enzymatic hydrolysis. We believe that wet storage systems may also present a unique opportunity to add value to the feedstock through chemical or biological pretreatment. In-storage pretreatments at ambient temperature and pressure but prolonged reaction times may lower pretreatment costs and provide better return for farmers. Our research investigates the ability of on-farm pretreatments with dilute acid, alkali, ozone or novel enzymes to improve enzymatic degradability of cellulose and hemicelluloses in biomass at the biorefinery.

## *Use of a Microbe to Mitigate Inhibitors in Biomass Fermentations*

**Thursday, September 30, 2010: 1:30 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Nancy N. Nichols, Bruce S. Dien, Badal C. Saha and Michael A. Cotta, Bioenergy Research Unit, National Center for Agricultural Utilization Research, USDA-ARS, Peoria, IL

The presence of inhibitory compounds in biomass sugars is a significant hurdle to conversion of biomass to fuels and chemicals. The fibrous nature of lignocellulosic biomass necessitates physical-chemical pretreatment to deconstruct plant cell walls and render cellulose accessible to enzymatic digestion. Pretreatment in turn generates inhibitory compounds that affect microbial cell membranes, macromolecular synthesis, and glycolytic and fermentative enzymes. Inhibitors, comprising furan aldehydes, organic acids, and aromatic aldehydes and phenolics, result in failed or extensively prolonged fermentations as microorganisms attempt to adjust their metabolism to cope with the inhibitors. The microbial inhibitors present in biomass hydrolysates must therefore be mitigated to enable efficient fermentations. The inhibitory compounds, however, can also serve as a source of carbon and energy for some microbes. To this end, a soil microbe was isolated by selective screening that is uniquely suited for mitigating fermentation inhibitors, by metabolizing inhibitory compounds present in biomass dilute acid hydrolysates. Biological abatement using the fungal isolate, *Coniochaeta ligniaria*, results in improved fermentability of pretreated sugar streams, compared to unconditioned hydrolysates. Bioabatement has been evaluated in fermentations of crop residues and potential energy crops, and is advantageous to other methods of inhibitor mitigation.

## *Protein Engineering of GRE2 From Saccharomyces Cerevisiae for Enhanced Detoxification of 5-Hydroxymethyl Furfural*

**Thursday, September 30, 2010: 2:00 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Jaewoong Moon and Z. Lewis Liu, Bioenergy Research Unit, National Center for Agricultural Utilization Research, USDA-ARS, Peoria, IL

Furfural and 5-hydroxymethylfurfural (HMF) are representative inhibitors generated by lignocellulosic biomass pretreatment such as dilute acid hydrolysis that inhibit microbial growth and subsequent fermentation. It is possible to in situ detoxify these inhibitory compounds using tolerant *Saccharomyces cerevisiae* through NAD(P)H-dependent aldehyde reductions. GRE2 is a commonly recognized up-regulated gene by stress conditions with reductase activities. Using a directed enzyme evolution approach, we engineered the genetic code of GRE2 yielding two mutants with amino acid substitutions of Gln261 to Arg261 and Phe283 to Leu283; and Ile107 to Val107, Gln261 to Arg261, and Val285 to Asp285 for Y62-C11 and Y62-G6, respectively. Clones of these mutants showed better growth rates and were able to establish viable cultures under 30mM HMF challenges as an initial inoculum when compared with a wild type GRE2 clone on a synthetic medium. The improved mutants displayed approximately 3- to 4-fold increase of specific enzyme reduction activity toward HMF, and a 3- to 9- fold increase to furfural compared with their parental wild type gene. Derivatives of *S. cerevisiae* NRRL Y-50049 transformed with these mutated genes demonstrated significantly higher levels of HMF-to-FDM conversion. In purified Y62-G6, aldehyde reductase activity toward furfural and HMF using NADPH was 13- to 15- fold increased compared with a wild type GRE2. Site directed mutagenesis and subsequent enzyme assay showed that the amino acid substitution of Asp at 285 affected cofactor preference for enhanced reduction activities.

# Process Efficiency Improvements

Thursday, September 30, 2010: 12:30 PM

Alumni Lounge (Illinois Institute of Technology)

## Description:

Process efficiency can be improved by adjusting process arrangement, applying new technology, using efficient device etc. As a result, the overall cost of operating or capital can be significant reduces. Sharing these technologies would be beneficial to companies, even whole nation. The Session is open to present any ideas, experiment results, industrial examples for improvements of process efficiency.

## Chair:

Zhijun Jia

Email: [zhijun.jia@chart-ind.com](mailto:zhijun.jia@chart-ind.com)

## Co-Chair:

Magali Ferrandon

Email: [ferrandon@anl.gov](mailto:ferrandon@anl.gov)

## *An Efficient Stochastic Optimization Framework for Studying the Impact of Seasonal Variation On the Minimum Water Consumption of Pulverized Coal (PC) Power Plants*

Thursday, September 30, 2010: 12:30 PM

Alumni Lounge (Illinois Institute of Technology)

Juan M. Salazar and Urmila Diwekar, Vishwamitra Research Institute, Center for Uncertain Systems: Tools for Optimization and Management, Clarendon Hills, IL

Coal-fired power plants are large water consumers second only to agricultural irrigation. Water restrictions become more influential when water-expensive carbon capture technologies are added to the process. Therefore, national efforts to study the reduction of water withdrawal and consumption in existing and future plants have been intensified. Water consumption in these plants is strongly associated with the dry bulb temperature and humidity of air. There is significant variability in these parameters. In this work, we characterized the uncertainty and variability in these parameters in terms of probability distributions. These distributions change with seasons. We obtained optimal operating conditions for each season in the face of uncertainties using water minimization as the objective. It has been found that the water consumption is reduced from 3.2 to 15.4 % depending on the season. In order, to solve this large scale real world optimization problem, we had to resort to an efficient stochastic nonlinear programming (SNLP) algorithm called Better Optimization of Nonlinear Uncertain Systems (BONUS). It has been found that BONUS reduces the computationally intensity of this problem by 98.7%, making it possible to obtain optimal operating conditions in reasonable computational time.

## *Process Efficiency for Regeneration of Ammonia Borane*

Thursday, September 30, 2010: 12:50 PM

Alumni Lounge (Illinois Institute of Technology)

Thanh Hua and Rajesh Ahluwalia, Nuclear Engineering Division, Argonne National Laboratory, Argonne, IL

Ammonia borane (NH<sub>3</sub>BH<sub>3</sub>, AB) is considered a promising hydrogen carrier for automotive fuel cell systems because of its high hydrogen density (19.6 wt%) and the exothermicity of the dehydrogenation reaction. Release of hydrogen from ammonia borane results in the formation of polyborazylene spent fuel, which must be processed off-board to recycle AB and close the fuel cycle. We have assessed the efficiency of three approaches of digesting the spent AB into intermediates and reducing them to AB: thiocatechol for digestion and tin metal hydride for reduction, tert-butanol for digestion and a metal hydride for reduction, and direct digestion and reduction by hydrazine in ammonia.

## *Structural Characterization and Theoretical Calculation of Furfuryl Alcohol and Hydroxymethylfurfural*

Thursday, September 30, 2010: 1:10 PM

Alumni Lounge (Illinois Institute of Technology)

Taejin Kim<sup>1</sup>, Rajeev Assary<sup>2</sup>, Larry Curtis<sup>2</sup>, Christopher Marshall<sup>3</sup> and Peter Stair<sup>3</sup>, (1)Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL, (2)Materials Science Division, Argonne National Laboratory, Argonne, IL, (3)Argonne National Laboratory, Argonne, IL

Levulinic acid derived from hydrolysis of Furfuryl alcohol and Hydroxymethylfurfural has found a useful range of applications in the liquid transformation fuel and potential chemical products. Although several liquid and solid acid catalysts have been studied in the presence of water and organic solvent, the fundamental elementary process studies involved in catalysis at surfaces in a liquid phase environment is in infancy. In order to establish the solid acid catalyst surface molecular structure and identify intermediate molecular species, in-situ spectroscopy techniques are needed. Raman spectroscopy is a powerful spectroscopic technique for characterizing molecular structure and has been applied to the study of chemistry, biology, and material science. To investigate the disclosed intermediate species, the molecular structure of the basic reactants and products information should be achieved. The aim of the present work was to carry out a spectroscopy technique and theoretical calculation to explore the fundamental understanding of the key molecular structures, HMF and FA, regarding of levulinic acid production. Further, to investigate the five member ring molecular structure vibrational frequencies, the two molecules furan and furfural were also selected and compared to HMF and FA. Furan, Furfural, Furfuryl alcohol (FA), Hydroxymethylfurfural (HMF), and Levulinic acid samples were obtained commercially from Sigma-Aldrich. The Raman spectra of the liquid samples were obtained with visible excitation (488nm:Princeton Instruments Acton, Tivista 555, 632.8nm:Reinshaw 2000 Raman Spectrometer) in the 100-4000 cm<sup>-1</sup> spectral region at a resolution of cm<sup>-1</sup>. The Reinshaw Raman spectrometer was equipped with an optical microscope (Leica DM) which was used in focusing. The visible excitation was generated by Argon Ion (488nm) and HeNe (632.8nm) laser and scattered photons were direct into a single monochromator/triplespectrograph and focused onto an air/liquid nitrogen cooled CCD detector. The laser power delivered to the sample was 10~15mW. The spectral acquisition time used was 5~10 scans of 10~20 seconds/scan. All visible Raman spectra were obtained at room temperature and ambient pressure. The geometries, zero-point energies, thermal energies were evaluated at B3LYP/6-31+G(2df,p) level of theory using Gaussian 03 software. All the enthalpies of the reactions are evaluated at G4 level of theory which is known to predict the thermochemistry of the gas phase reactions with chemical accuracy.

## *Pressurized Steam Reforming of Bio-Derived Fuels for Distributed Hydrogen Production – A Systems Model Analysis to Compare System Efficiency*

**Thursday, September 30, 2010: 1:30 PM**

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Dionissios D. Papadias, Sheldon Lee and Shabbir Ahmed, Argonne National Laboratory, Chicago, IL

Light-duty fuel cell vehicles are being developed by many automobile manufacturers. One of the strategies for refueling these vehicles is to set up distributed hydrogen production facilities – small plants located at the refueling stations that will convert bio-derived fuels to high-purity hydrogen, where the hydrogen will be produced by the steam reforming of the bio-derived fuel. The hydrogen will then be purified by pressure swing adsorption (PSA). These processes would typically be designed to produce high-purity hydrogen at pressures of 8–20 atm (118–295 psi), which will subsequently be compressed and delivered to the vehicle at pressures of 340–680 atm (5,000–10,000 psi). Compressing the hydrogen to such high delivery pressures requires a considerable amount of electrical energy. Depending on the initial pressure at which the hydrogen is available, this compression energy requirement can represent a significant percentage of the lower heating value (LHV) of the product hydrogen (20% from 20 to 340 atm), assuming that the thermal energy efficiency to produce the electricity is 34%.

We will present the results of our system analysis study for the steam reforming of bio-derived ethanol at elevated pressures. The objective of this work is to examine the option of using Pd-membrane technology for the separation of hydrogen. The relative merits of one or more promising scenarios will be presented with respect to their potential for meeting the DOE efficiency targets for producing hydrogen from bio-derived liquid fuels. The study compares the efficiencies achievable by Pd-membrane based reactor system to those of reference systems with non-membrane reactors. Examples of the effects of changes in system design (layout, hydrogen flux, etc.) and operating conditions (temperature, pressure, steam-to-carbon ratio, etc.) on the efficiency of hydrogen production will be presented.

## *Compact Heat Exchange Reactor In Fischer-Tropsch Process Application*

**Thursday, September 30, 2010: 1:50 PM**

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Zhijun Jia and Larry Stryker, Chart Energy & Chemicals, La Crosse, WI

Chart's compact heat exchange reactor has been used in various applications to improve process efficiency and safety, especially for highly exothermic or endothermic reactions. FT reaction is one of the examples. The reactor consists of multiple layers for reaction and cooling which are alternatively arranged. Each reaction layer contains multiple mini-channels in is in mm scale. Catalysts are packed into those mini-channels. The tested reactor is made of aluminum which provides an excellent heat transfer character. The operating conditions are up to 230C at 20 bars. The reactors were continuously running the reactor for three weeks. The results indicated that the compact heat exchange reactor provided unique features to improve the process efficiency and productivity.

## *Vibrational Properties of Levulinic Acid and Furan Derivatives: Raman Spectroscopic and Theoretical Calculation*

**Thursday, September 30, 2010: 2:10 PM**

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Taejin Kim<sup>1</sup>, Rajeev Assary<sup>2</sup>, Larry A. Curtiss<sup>2</sup>, Christopher L. Marshall<sup>1</sup> and Peter C. Stair<sup>3</sup>, (1)Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL, (2)Materials Science Division, Argonne National Laboratory, Argonne, IL, (3)Department of Chemistry, Northwestern University and Chemistry Division, Argonne National Laboratory, Argonne, IL

The Raman spectra of furan, cis/trans furfural, furfuryl alcohol (FA), cis/trans hydroxy-methyl-furfural (HMF), and levulinic acid were investigated at room temperature. Peaks assignment was assisted by B3LYP/6-31+G(2df,p) density functional theory. Agreement between theoretically calculated vibrational frequencies and measured spectra was good, while calculated spectra for furan and furan derivatives showed overestimated C-H stretching peak intensity. The Raman frequency at 1470 ~ 1500 cm<sup>-1</sup>, C=C double bonds stretching frequencies, were consistent for all furan derivatives. Both Furfuryl alcohol and HMF were very stable and found that do not undergo hydrolysis to form levulinic acid in neutral conditions. An aqueous FA solution formed the dark solids with sulfuric acid and characterized by Raman spectrometry. The characterization results implied that the dark solids mainly consisted of carbon.

# Renewable Biofuels From Lignocellulose - Recent Advances II

Thursday, September 30, 2010: 3:00 PM  
Armour Dining (Illinois Institute of Technology)

## Description:

The Energy Independence and Security Act of 2007 seeks to expand biofuel production to 36 billion gal/yr by 2022 to replace 20% of our gasoline and targets at least 60% to be advanced biofuels including those produced from lignocellulose. Lignocellulose is an abundant, low-cost, non-food, non-feed feedstock for the production of biofuels. It is available in the form of crop waste matter, such as corn stover, dedicated bioenergy crops, such as switchgrass or Miscanthus, and municipal and forestry wastes. However, significant technical challenges must be overcome to achieve cost-competitive conversion of these feed-stocks. The fibrous cell-wall material that constitutes lignocellulosic feed-stocks is difficult to deconstruct and depolymerize into fermentable sugars. The pretreatment required to open the structure to subsequent enzymatic hydrolysis tends to result in dilute solutions of hexose and pentose sugars containing inhibitors that deter subsequent fermentation to biofuel by microorganisms. Advancements in pretreatments, enzymes and microorganisms to improve resilience, efficiency and cost-effectiveness are emerging. These are being incorporated into processes to be optimized for economical biofuel production from lignocellulose. Progress in this area promises to meet national priorities to reduce dependence on foreign oil, lower greenhouse gas emissions, and promote the rural economy. Presentations will emphasize recent advancements in biocatalytic tools and processes for production of biofuels from lignocellulose.

## Chair:

Patricia J. Slininger

Email: [Pat.Slininger@ars.usda.gov](mailto:Pat.Slininger@ars.usda.gov)

## *Reprogrammed Glucose Metabolic Pathways of Inhibitor-Tolerant Yeast*

Thursday, September 30, 2010: 3:00 PM

[Armour Dining \(Illinois Institute of Technology\)](#)

Z. Lewis Liu, Menggen Ma and Michael A. Cotta, Bioenergy Research Unit, National Center for Agricultural Utilization Research, USDA-ARS, Peoria, IL

Representative inhibitory compounds such as furfural and 5-hydroxymethylfurfural generated from lignocellulosic biomass pretreatment inhibit yeast growth and interfere with the subsequent ethanol fermentation. Evolutionary engineering under laboratory settings is a powerful tool that can be used to generate valuable strains and knowledge for inverse metabolic engineering for strain improvement. An inhibitor-tolerant ethanologenic yeast *Saccharomyces cerevisiae* developed via evolutionary engineering underwent a genomic adaptation with global integrations for acquired tolerant functions while producing ethanol. Gene expression data provide informative phenotypes and significant insight into molecular mechanisms of the tolerance in yeast. Unification of gene expression data analysis is urgently needed to efficiently utilize the massive amount of data resource from individual research efforts as well as for the expression community in general. A rigorously tested and validated pathway-based real time qRT-PCR array assay applying robust mRNA reference and a master equation provide reliable means for reproducible and comparable expression data analysis. Advances in enhanced expression technology has led to discoveries of new gene functions and interactions to form hypothesis and construct reprogrammed pathways for the tolerant yeast in response to the inhibitor stress. Enriched genetic makeup, continued enhanced expression of genes in maintaining energy and redox balance, and the reprogrammed glucose metabolic pathways globally enable the yeast tolerance. Findings of recent research aid understanding of molecular mechanisms of stress tolerance and guide metabolic engineering efforts for future robust strain development to support biofuels industry.

## *Process Design Considerations for Optimal Production of Ethanol From Lignocellulose Using Available Yeasts, Including Natural Pentose-Fermenting Yeasts, and Their Derivatives*

**Thursday, September 30, 2010: 3:30 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Patricia J. Slininger, Bioenergy Research Unit, National Center for Agricultural Utilization Research, Peoria, IL, Jaewoong Moon, Biological Systems Engineering, National Center for Agricultural Utilization Research, USDA-ARS, Peoria, IL and Z. Lewis Liu, Bioenergy Research Unit, National Center for Agricultural Utilization Research, USDA-ARS, Peoria, IL

To expand the biomass to fuel ethanol industry, process strategies are needed to foster the production and utilization of microorganisms which can survive and ferment both hexose (C6) and pentose (C5) sugars while exposed to inhibitors (such as ethanol, furfural, and hydroxymethylfurfural, or HMF). Furfural and HMF are key byproducts of biomass pretreatment procedures to allow efficient enzymatic release of fermentable sugars during the hydrolysis of lignocellulose. The conversion of five-carbon xylose to ethanol and the inhibitor tolerance of the natural pentose-fermenting yeast *Scheffersomyces (Pichia) stipitis* NRRL Y-7124 has been optimized using a culture medium that supplied sufficient minerals and nitrogen as a mixture of urea and amino acids. During hydrolyzate fermentation, the switch from glucose to xylose uptake can result in diauxic lag unless steps are taken to prevent this. Priming yeast populations with a high xylose concentration was observed to induce faster fermentation rates in ethanol production fermentors and to eliminate diauxic lag during mixed sugar conversion by recycled *S. stipitis* populations. Ethanol concentrations circa 50 g/L have been found to repress induction of enzymes required for xylose-utilization. The process strategy of recycling xylose-primed cells was key to successful rapid utilization of high mixed sugar concentrations because specific enzymes for xylose utilization were induced before ethanol concentration climbed to an inhibitory level that would prevent xylose uptake. Using nutrition, culture priming, and cell recycle technologies, *S. stipitis* Y-7124 yields an economically recoverable 66 g/L ethanol in 48 h at a conversion efficiency of 88% (0.44 g ethanol/g sugar) from 95 g/L of glucose and 55 g/L xylose in defined media. Recent results of the application of these process strategies to the fermentation of lignocellulosic process streams in order to produce economically recoverable ethanol from biomass will be described.

## *Novel Developments in Butanol Fermentation: Microbial Genetics to Agricultural Substrates, Process Technology, and Downstream Processing*

**Thursday, September 30, 2010: 4:00 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Nasib Qureshi<sup>1</sup>, Siqing Liu<sup>2</sup>, Badal C. Saha<sup>1</sup> and Michael A. Cotta<sup>1</sup>, (1)Bioenergy Research Unit, National Center for Agricultural Utilization Research, USDA-ARS, Peoria, IL, (2)Renewable Product Technology Research, National Center for Agricultural Utilization Research, USDA-ARS, Peoria, IL

Butanol is the major product of acetone-butanol-ethanol (ABE; ratio 3:6:1) fermentation. It can be produced from various carbohydrates such as glucose, corn, molasses, and whey permeate (a by-product of dairy industry) using microbial strains such as *Clostridium beijerinckii* and/or *C. acetobutylicum* in batch reactors. This chemical can be used as a feedstock or biofuel and contains more energy than ethanol on a weight basis. The maximum concentration of ABE in a batch reactor is limited to 20-30 g/L due to end product inhibition. At that concentration, growth and fermentation of the microbial strain are completely arrested. In an attempt to commercialize this fermentation, economic studies were performed on the use of agricultural residues as substrates in addition to the application of process technology and energy efficient recovery from the fermentation broth. As a result of these studies, we investigated the use of wheat straw, corn stover, barley straw, and switchgrass as economical substrates. The cost of these substrates has been projected to be \$24-60 per ton. Unfortunately, fermentation of some of these substrates (barley straw, corn stover and switchgrass) is difficult due to generation of inhibitors during pretreatment and hydrolysis. We successfully removed inhibitors from barley straw and corn stover hydrolyzates by overliming them and fermented the detoxified sugar mixture (hexoses and pentoses) successfully. We were also successful in developing an integrated process for the production of butanol from wheat straw. In this process hydrolysis, fermentation, and ABE recovery were combined. The new process was called simultaneous saccharification, fermentation, and recovery (SSFR). In such an integrated process product (ABE) concentration in the reactor was kept below 10 g/L (to avoid product inhibition) while in the recovered stream product level

reached over 70 g/L. We also developed butanol producing lactic acid bacterial (LAB) strains such as *Lactococcus lactis* and *Lactobacillus buchneri*. Some of the LAB strains are butanol tolerant and can grow in up to 30 g/L butanol solution. The results of these investigations will be presented.

## *Optimal Control of Biodiesel Production In a Batch Reactor In the Face of Feed Variability*

**Thursday, September 30, 2010: 4:30 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Pahola T. Benavides, VRI- Custom, Chicago, IL and Urmila Diwekar, Vishwamitra Research Institute, Center for Uncertain Systems: Tools for Optimization and Management, Clarendon Hills, IL

The depletion of the fossil fuel reserves and the increasing environmental concerns encourage engineers and scientists to look for an alternative, clean and renewable fuel that can reduce environmental impact. Biodiesel has been considered as the best candidate of one of these renewable fuels. One of the pathways to biodiesel production is the transesterification reaction of triglycerides from vegetable oils and short-chain alcohols. A batch reactor is employed for production of biodiesel. The flexibility of the process allows operating the reactor with completely different feed stock and product specifications. This condition becomes challenging for the reactor modeling and control since uncertainty in the feed composition turn into time-dependent uncertainty and requires a batch-process stochastic optimal control. In this work, the uncertainties resulting from the variation of feed stock composition are quantified, characterized and propagated through the model. Generated time-dependent uncertainties are modeled using Ito processes. The optimal control in this reactor involves optimization of the yield of fatty acid methyl esters, well known as biodiesel, under control of reactor temperature and the strategy applied to solve this problem is based on stochastic maximum principal and shooting approach.

# **Petroleum Refining - Factoring in Reliability**

**Thursday, September 30, 2010: 3:00 PM**  
Trustee Room (Illinois Institute of Technology)

## **Description:**

Equipment reliability continues to be an important aspect of refinery operations. Companies are devoting an increasing number of resources to analyze processes to improve the long-term reliability of equipment. This session will address aspects of refinery operations that affect equipment reliability and improved methods of process analysis. In addition, several examples of refinery failures will be discussed and the oil industry's approach to human aspects of reliability will be reviewed.

## **Chair:**

Ranti Ihimoyan

**Email:** [aogunri@citgo.com](mailto:aogunri@citgo.com)

## **Co-Chair:**

Jerry Wilks

**Email:** [gwilks@citgo.com](mailto:gwilks@citgo.com)

## *High Acid Crude Processing: Corrosion Control Strategies*

**Thursday, September 30, 2010: 3:00 PM**

[Trustee Room \(Illinois Institute of Technology\)](#)

Randy Rechten, 2929 Allen Parkway, Suite 2100, Baker Hughes, Houston, TX

As refiners continue to process heavier, more acidic crude blends, there is a corresponding need to properly address increased corrosion activity in the Crude Unit. In particular, today's refiners face serious challenges from naphthenic acid corrosion in atmospheric and vacuum gas oils and resids. Troubleshooting naphthenic acid corrosion requires detailed knowledge of both the mechanisms involved as well as the proper mitigation steps required. Many techniques are available to better understand these corrosive effects, including metallurgical analysis, hydrogen permeation measurements and molecular analysis of inhibited scale layers. In addition, a thorough understanding of the refinery system must include an assessment of the areas at risk for corrosion and calculation methods for correctly determining velocity/shear effects in mixed phase flow regimes. Details of these troubleshooting strategies will be presented along with examples from field applications.

## *Risk Management of High Temperature Refinery Equipment*

**Thursday, September 30, 2010: 3:30 PM**

[Trustee Room \(Illinois Institute of Technology\)](#)

Peter Carter, Chris Matice and Claudio Allevato, Stress Engineering Services, Wheeling, IL

The paper will summarize the scope and some limits of current fitness-for-service (FFS) methods and focus on selected areas where there are prospects for improvement in refinery equipment analyses. The examples are high temperature weld assessment, accelerated post-exposure testing and advanced monitoring methods such as acoustic emission. These methods have the potential to alter certain limitations in current methods arising from approximate analysis methods and scatter in the basic material data. This usually forces assessments to be based on worst case and unrealistic load and material combinations and on "minimum" data and which can lead to errors associated with excessive conservatism. Inspection is a part of an FFS program, and one of the challenges is insulated high energy girth welded piping systems. Acoustic emission monitoring has been used to identify changes for piping weld characteristics, signaling the need for closer investigation.

## *Reliability Planning & Execution In Refining Projects*

**Thursday, September 30, 2010: 4:00 PM**

Trustee Room (Illinois Institute of Technology)

Tom Brindley and Mike Hammond, CITGO Petroleum Corporation, Lemont, IL

The CITGO Petroleum Corporation's refineries in Lemont, IL and Corpus Christi, TX, have integrated new units into the respective refineries to produce ultra low sulfur diesel. The projects were configured so that a single design could be used to build two nearly identical units that required some of the largest equipment in the industry. The combined mega-project was executed during one of the most severe market swings in refining history. Simultaneously, suppliers to the industry are outsourcing and off-shoring more critical activities and components more than ever with varying degrees of oversight on their sub-suppliers. This combination creates significant challenges to ensuring the reliability of a new process unit. The presentation will identify some of the engineering details and managerial methods employed to ensure reliability. Some of the problems that were encountered such as material quality and control, packaged equipment integration, instrumentation selection, and overall craftsmanship will be discussed. Finally, proposed methods in design and execution to ensure reliability on future projects will be explored.

# Integrated Renewable Systems for a Green (\$) Economy

Thursday, September 30, 2010: 3:00 PM  
Alumni Lounge (Illinois Institute of Technology)

## Description:

Access to clean energy and water in nations and communities worldwide who aim to achieve sustainable development is among the top challenges of this century. In addition, the global interest in renewable energy technologies has peaked over the past few years due to escalating energy prices and mounting public concern over the environment. Another emerging challenge is the continued dependence on foreign sources of energy which causes a threat to national energy security. Papers presented in this session will address these urgent issues.

## Chair:

Sohail Murad

Email: [murad@uic.edu](mailto:murad@uic.edu)

## Co-Chair:

Said Al-Hallaj

Email: [salhallaj@allcelltech.com](mailto:salhallaj@allcelltech.com)

## *Clean and Renewable Energy Policy and Program Recommendations*

Thursday, September 30, 2010: 3:00 PM

Alumni Lounge (Illinois Institute of Technology)

Suzanne Malec-McKenna, Chicago Department of Environment, Chicago, IL and  
Howard Learner, Environmental Law & Policy Center Chicago Climate Action Plan

## *The Carbon and Energy Footprint of Water Treatment, Distribution and Reclamation and Waterway Management In Greater Chicago*

Thursday, September 30, 2010: 3:30 PM

Alumni Lounge (Illinois Institute of Technology)

Pete Mulvaney<sup>1</sup>, Catherine A. O'Connor<sup>2</sup>, Antonio Quintanilla<sup>2</sup>, Louis Kollias<sup>2</sup>, Manju Sharma<sup>2</sup> and Richard Lanyon<sup>2</sup>, (1)Metropolitan Water Reclamation District of Greater Chicago, Chicago, IL, (2)Research and Development, Metropolitan Water Reclamation District of Greater Chicago, Cicero, IL

## *The Emerald Forest– Algae Production In a Pilot-Scale Photobioreactor*

Thursday, September 30, 2010: 4:00 PM

Alumni Lounge (Illinois Institute of Technology)

Fouad Teymour, Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, IL

## *Heat Recovery at a Water Reclamation Plant In Greater Chicago*

Thursday, September 30, 2010: 4:30 PM

Alumni Lounge (Illinois Institute of Technology)

Ali K. Oskouie, Catherine A. O'Connor, David Lordi, Louis Kollias and Richard Lanyon, Research and Development, Metropolitan Water Reclamation District of Greater Chicago, Cicero, IL

## **General Poster Session**

**Thursday, September 30, 2010: 5:00 -7:30 PM**  
Expo Room (Illinois Institute of Technology)

**Description:**

This poster session welcomes contributions on topics of interest in chemical engineering research and development. A separate program listing of poster titles, authors and abstracts will be provided at the poster session.

**Chair:**

Justin M. Notestein

**Email:** [j-notestein@northwestern.edu](mailto:j-notestein@northwestern.edu)

# Perfect Power Implementation, Education, and Research at the Illinois Institute of Technology

Friday, October 1, 2010: 9:30 AM  
Trustee Room (Illinois Institute of Technology)

## Description:

Refer to the “Perfect Power Implementation at Illinois Institute of Technology” Abstract.

## Chair:

Mohammed Shahidehpour

Email: [ms@iit.edu](mailto:ms@iit.edu)

## *Perfect Power Implementation at Illinois Institute of Technology*

Friday, October 1, 2010: 9:30 AM  
Trustee Room (Illinois Institute of Technology)  
Joseph Clair, Illinois Institute of Technology, Chicago, IL

The Perfect Power project has several goals in three categories: technical, financial and leadership. The technical goals include the demonstration of the key capabilities of Perfect Power with respect to reliability, demand response load reduction, energy efficiency load reduction and integration of renewable sources. The financial goals include the deferral of major capital costs, the reduction of energy and outage costs, as well as the influx of ancillary services' revenues. The leadership goals include the reduction of the university's carbon footprint, the creation of a living laboratory and the opportunity to lead Smart Grid development through the Perfect Power project. This presentation will highlight the listed issues.

## *Autonomous Agents for Advanced Distribution Automation In Perfect Power Systems*

Friday, October 1, 2010: 10:00 AM  
Trustee Room (Illinois Institute of Technology)  
Alex Flueck, Electrical and Computer Engineering, Illinois Institute of Technology, Chicago, IL

Autonomous agents have the potential to revolutionize the operation of distribution systems. Advanced distribution automation strategies, such as fault detection, location and isolation, as well as restoration, reconfiguration and volt/VAR management can be improved via autonomous agents. The Perfect Power System at IIT has implemented an agent-based control system, known as the High Reliability Distribution System (HRDS). In addition, IIT researchers are creating new agent-based technologies for advanced distribution automation. Join us for a presentation on agent-based solutions, including a brief demonstration of the IIT distribution system simulator and visualization platform.

## *Update on IIT Microgrid Master Controller*

**Friday, October 1, 2010: 10:30 AM**

[Trustee Room \(Illinois Institute of Technology\)](#)

Greg Rouse, Intelligent Power Solutions, Santa Ana, IL

IIT has commissioned Intelligent Power Solutions to develop microgrid master controller software for the campus. The purpose of the master controller is to coordinate the control of energy systems at the campus in response to external influences such as the quality of the local grid supply, weather conditions, electricity market prices and demand response events. IIT's energy systems consist of 6MW of gas turbines, building load controllers and the campus's automated electrical distribution system. These systems have existed independently for years but have typically operated independently of each other with only manual interaction between them. Examination of some of the issues with IIT's distribution system, systems thinking, and increased interest in microgrids have made the benefits of a coordinated microgrid much more obvious. The master controller will help the campus take actions to respond to these conditions with the goals of maximizing reliability, savings, energy security, efficiency and carbon reduction. Mr. Rouse will present an introduction of IIT's microgrid master controller and an update on the status of its development.

## *Application of Zigbee Wireless In Smart Grid*

**Friday, October 1, 2010: 11:00 AM**

[Trustee Room \(Illinois Institute of Technology\)](#)

Chi Zhou, ECE Department, Illinois Institute of Technology, Chicago, IL

The smart grid is an intelligent power generation, distribution and control system. ZigBee, as wireless mesh networking scheme low in cost, power, data rate, and complexity, is ideal for smart grid applications for real-time system monitoring, load control, and building automation.

However, many issues need to be addressed when applying Zigbee wireless to smart grid, including coexistence with other technologies, energy efficient MAC and routing protocols, interoperability, scalability, etc. In this talk, we focus on one issue, developing practical Zigbee deployment guideline under WLAN interference. We identify the "Safe Distance" and "Safe Offset Frequency" using a comprehensive approach including theoretical analysis, software simulation, and empirical measurement. In addition, we propose a frequency agility-based interference avoidance algorithm. The proposed algorithm can detect interference and adaptively switch nodes to "safe" channel to dynamically avoid WLAN interference with small latency and small energy consumption. Our proposed scheme is implemented on a Meshnetics ZigBit Development Kit and its performance is empirically evaluated in terms of the packet error rate (PER) using a ZigBee and Wifi coexistence testbed. It is shown that the empirical results concur with our analytical results and our design guideline can efficiently mitigate the effect of WiFi interference and enhance the performance of Zigbee networks.

## *Illinois Institute of Technology Smart Grid Education and Workforce Training Center*

**Friday, October 1, 2010: 11:30 AM**

[Trustee Room \(Illinois Institute of Technology\)](#)

Melissa Gordon, IIT Smart Grid Education and Workforce Training Center, Illinois Institute of Technology, Chicago, IL

In April 2010, the Illinois Institute of Technology won a competitive grant award from the Federal Department of Energy to establish a World-Class Smart Grid Education and Workforce Training Center. The Center's mandate is to develop and deploy Smart Grid technology courses and certificate programs via classroom and distance-learning methodologies that will have both a local and global impact. The Center will use the Illinois Institute of Technology's strong and already established Smart Grid and power engineering infrastructures to engage utilities, corporations, Labor Unions, K-12 students and educators, Veterans, and universities and community colleges in a collaborative initiative to train the strongest workforce in the world to meet the global challenges in Smart Grid, energy independence, clean environment, and sustainable energy.

# Process Safety Developments

Friday, October 1, 2010: 9:30 AM

Alumni Lounge (Illinois Institute of Technology)

## Description:

Statistically, the chemical process industry is a relatively safe place to work. However, the industry does occasionally suffer a catastrophic accident as well as more numerous, lesser events. Many industry and regulatory initiatives, as well as research and technical modeling developments, have occurred in recent years with the goal of reducing these losses. The papers in this session offer a view of some of these efforts that have applicability across the broad range of facilities in which chemical engineers operate, and are intended to be of interest to anyone involved in the design or operation of a chemical processing facility.

## Chair:

Mike Moosemiller

Email: [mmoosemiller@bakerrisk.com](mailto:mmoosemiller@bakerrisk.com)

## *Materials Signature of Fires*

Friday, October 1, 2010: 9:30 AM

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Robert O'Shea Jr., Baker Engineering and Risk Consultants, Inc., Chicago, IL

There are 50 some different metals. However, in ordinary use in households and industrial building, there are basically five types of metals:

1. steel,
2. cast irons,
3. copper,
4. aluminum and
5. zinc

Each has unique properties, strengths, color, and reaction to fire, temperature, and the environment of a fire. This talk will present information about fires from a materials point of view. Specific examples from specific fire investigations will be presented.

## *Safety Critical Instrumentation Testing Guidelines*

Friday, October 1, 2010: 10:00 AM

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Peter G. Herena, Kenexis Consulting Corporation, Elgin, IL and Yasser Ali Khalil, ZADCO

The widespread adoption of the IEC/ISA 61511 standard for safety instrumented systems along with the utilization of Layer of Protection Analysis (LOPA) has focused a lot of attention on assuring the mechanical integrity of instrumented safeguards in the process industries. This presentation reviews the design guidelines for non-Safety Instrumented System Independent Protective Layers and proposes an extension of those standards using IEC/IEC 61511 style analysis to determine the most appropriate testing intervals for those functions. In addition, the presentation includes a table of "typical" test intervals for common instruments that will allow the discussed performance targets to be achieved.

## *Guide to Developing and Implementing Safety Checklists: Plant Steam Utilities*

**Friday, October 1, 2010: 10:30 AM**

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Juan C. Ramirez<sup>1</sup>, Mark Fecke<sup>1</sup>, John Martens<sup>2</sup> and Delmar "Trey" Morrison<sup>3</sup>, (1)Exponent, Lisle, IL, (2)Exponent, Inc., Lisle, IL, (3)Exponent, Inc., Wood Dale, IL

Steam generation is an integral part of most chemical process plants; however, the steam plant can be overlooked in the area of hazard analysis. The reasons for this oversight are obvious: steam generation is considered to be an old and well understood process, and steam boiler systems are often not considered to pose the same hazards as other plant units. However, modern steam boiler systems are fueled with natural gas, pulverized coal, and/or fuel oil; each of which poses significant fire and explosion hazards. Chemical plants rely upon equipment design and installation, maintenance practices, operating procedures, and programmable logic controllers (PLCs) to operate safely. Steam plants are no different.

A hazard analysis technique that we have found useful to apply to these systems is that of a safety checklist based upon relevant standards and good engineering practice. More than just identifying the hazards and required safeguards for such a system, if implemented effectively, the checklist will enhance training and staff knowledge of boiler operation and safety systems. This paper aims to provide guidelines and hurdles in developing such a checklist.

## *Considerations for Relief System Design of Reactive Chemical Systems*

**Friday, October 1, 2010: 11:00 AM**

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Amy Theis, Fauske & Associates, LLC, Burr Ridge, IL

Guidelines for identifying an appropriate basis for the pressure relief system design of reactive chemical systems.

# Energy and the Environment

Friday, October 1, 2010: 9:30 AM

Armour Dining (Illinois Institute of Technology)

## Description:

Fossil fuels including coal, natural gas, and petroleum provide most of the energy used and at the same time impact the environment on a global scale. Achieving sustainable and secure energy use requires that energy be developed from Low to Zero Carbon sources. Energy needs to be produced by cleaner and more efficient technologies, and be used more efficiently and with greater conservation. The session examines the programs that are currently in place to reduce emissions, promote energy efficiency, and improve environmental quality without disrupting energy supplies

## Chair:

Kevin Taylor

Email: [k2356@aol.com](mailto:k2356@aol.com)

## *1. Study of Absorption Based Carbon Capture In a Coal Fired Power Plant*

Friday, October 1, 2010: 9:30 AM

[Armour Dining \(Illinois Institute of Technology\)](#)

Prakash Kotecha and Urmila Diwekar, Vishwamitra Research Institute, Center for Uncertain Systems: Tools for Optimization and Management, Clarendon Hills, IL

Coal based power generation has been an integral part of the energy portfolio of many countries. In United States, nearly half the electricity produced is generated from coal fired power plants. The huge coal reserves in a vast number of countries (including the US) supplemented by the immense expertise in safely operating such plants makes them an ideal candidate for enhancing the energy security of a nation. However, these plants also constitute as the second largest emitter of greenhouse gases. Nevertheless, the emissions from these power plants by their inherent stationary nature and large quantity provide an opportunity to employ viable carbon capture techniques thereby mitigating its effects on the global warming. Among the various techniques that have been considered for the capture of carbon di oxide, absorption has been found to be the most efficient and commercially viable technique. The capture of carbon di oxide using absorption based techniques has been quite prevalent in industries but not to the magnitude of the amounts of flue gases released from a standard power plant. Moreover, these absorption based carbon capture techniques can be conveniently retrofitted into an existing power plant without requiring major modifications in the upstream section of the plant. In this article, we have built a power plant model integrated with an absorption based carbon capture unit in ASPEN. This model has been used to study the various factors influencing the performance of an absorption based carbon capture system.

## *Characterization and Stochastic Modeling of Uncertainties In the Biodiesel Production*

Friday, October 1, 2010: 10:00 AM

[Armour Dining \(Illinois Institute of Technology\)](#)

Urmila Diwekar, Vishwamitra Research Institute, Center for Uncertain Systems: Tools for Optimization and Management, Clarendon Hills, IL and Sheraz Abbasi, Bioengineering, University of Illinois at Chicago, Chicago, IL

There are inherent uncertainties in the biodiesel production process arising out of feedstock compositions, operating parameters and mechanical equipment design and can have significant impact on the product quality and process economics. The uncertainties are quantified in the form of probabilistic distribution function. Stochastic modeling capability is implemented in the ASPEN process simulator to take into consideration these uncertainties and the output is evaluated to determine impact on plant efficiency.

## *Potential Impacts of PHEVs on Regional Power Systems*

**Friday, October 1, 2010: 10:30 AM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Jianhui Wang, Decision and Information Sciences Division, Center for Energy, Environmental, and Economic Systems Analysis, Argonne, IL and Cong Liu, Center for Energy, Environmental, and Economic Systems Analysis, Argonne, IL

In this talk, we will investigate the potential impact of high penetration of PHEVs on regional power systems. We will use several regions in the U.S. as case studies. We will discuss the impact of PHEVs on generation dispatch and planning, emission, and electricity prices.

## *An Overview of the Energy-Water Nexus*

**Friday, October 1, 2010: 11:00 AM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Leslie Poch, Environmental Science Division, Argonne National Laboratory, Argonne, IL

Water use in electric power generators is a critical issue not only in the United States but also the world. Droughts in this country have already forced some power plants to curtail generation or shutdown for periods of time. It is expected to get worse in the future. This presentation will discuss issues related to water usage in electric power generation and discuss work Argonne National Laboratory and others are doing to quantify the effects of water shortages on power generation. Strategies to reduce the threat of water resource limitations on electric power generation will also be discussed.

## *Collaboration and Technology Usher In the Era of Shale Gas*

**Friday, October 1, 2010: 11:30 AM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Trevor Smith, Gas Technology Institute (GTI), Des Plaines, IL

The world has within its grasp the possibility of realizing energy security, economic prosperity and environmental sustainability on a national, regional and global scale by understanding and utilizing our vast shale and other unconventional gas resources. The key to unlocking gas shales, tight gas sands and coal-bed methane (CBM) has been and continues to be collaboration and advanced technology, which enable the identification, development and deployment of solutions that reduce the risks and costs of production and minimize the environmental footprint of developing these vital resources.

## Process Industry Practices

Friday, October 1, 2010: 1:00 PM

Alumni Lounge (Illinois Institute of Technology)

### Description:

Engineering firms are increasingly called on to provide safe, efficient designs for an expanding variety of process industries facilities. These projects in the traditional petroleum refining, chemical manufacturing, food and pharmaceutical industries. Also, there are requirements for good, sustainable design of emerging biotechnology, nanotechnology and renewable energy plants. Today's presentations give just a hint of the types of problems design engineers solve and some of the tools which might be used to minimize engineering costs while maximizing design safety, quality and efficiency.

### Chair:

Jeff Kitz

Email: [Kitzgt@Middough.com](mailto:Kitzgt@Middough.com)

### *A Breakthrough In Flue Gas Cleanup, CO2 Mitigation and H2S Removal*

Friday, October 1, 2010: 1:00 PM

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Wolf Koch, Swapsol Corporation, Monmouth Junction, NJ

SWAPSOL Corp. is developing commercial processes around a newly discovered chemical reaction verified to reduce hydrogen sulfide (H<sub>2</sub>S) below detectable levels while reacting with carbon dioxide (CO<sub>2</sub>) to form water, sulfur and carsums, a carbon-sulfur polymer. The Stenger-Wasas Process (SWAP) stands to fundamentally simplify sulfur removal technology as it consumes carbon dioxide in an exothermic reaction under relatively mild process conditions. The SWAP will have applications in landfill gas, sour gas, flue gas cleanup, Claus tail gas cleanup and may serve as an alternative to Claus technology. A related process allows for the destruction of waste hydrocarbons to form hydrogen sulfide and carsums, providing a hydrogen sulfide source where it is not otherwise available. The primary reactions and variants have been independently verified and the chemical kinetics determined by a third party laboratory. Swapsol has filed US and international patent applications covering all aspects of the technology. Laboratory scale development of the various Swapsol processes is nearing completion and the company is exploring opportunities for pilot plant programs later this year.

### *Beryllium and Modern Day Alchemy*

Friday, October 1, 2010: 1:30 PM

[Alumni Lounge \(Illinois Institute of Technology\)](#)

Paul Jahn, Middough, Oak Brook, IL

Desired improvements in the economics and performance of many specialty metals today have become increasingly dependent on significant advances in chemical processes. This presentation introduces the unique role that beryllium plays in our national defense and the space industry while simultaneously providing an overview of a complex project underway in Northwestern Ohio to return production of this strategic metal to American soil. The key technology and execution challenges of this project will be discussed along with insights gained for engineers involved in similarly complex projects that cross multiple discipline boundaries.

# Modeling, Supervision and Control of Chemical, Biological and Pharmaceutical Processes

Friday, October 1, 2010: 1:00 PM

Armour Dining (Illinois Institute of Technology)

## Description:

Recent developments in modeling, supervision and control of various processes will be presented by researchers to provide an overview of research trends in these fields. Challenges in supervision and control of complex and distributed processes will be illustrated.

## Chair:

Ali Cinar

Email: [cinar@iit.edu](mailto:cinar@iit.edu)

## *Control of Complex Systems with Applications to Polymerization Reactors*

Friday, October 1, 2010: 1:00 PM

Armour Dining (Illinois Institute of Technology)

Fouad Teymour, Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, IL

The study of complex systems under the banner of complexity theory has demonstrated some fascinating properties that these inherently possess, and some interesting phenomena that emerge from their dynamic interaction, and has led to the discovery of new universality classes that span across all disciplines.

Armed with this heightened level of understanding the research community is contemplating the taming of these systems for the service of human society, an effort usually referred to as “*Building Engineered Complex Systems*.” As the name suggests this activity entails the transition from the stage of observation of complexity to that of systematic design aimed at harnessing its power and directing it towards the accomplishment of defined global objectives.

Naturally, process control and design will play an important role in this regard, but need to espouse new paradigms. Two of these paradigms, namely distributed/networked manufacturing and agent-based control, are discussed in detail in this presentation. We start with the question: “What does control of a complex system mean?” and end at applications in reactor networks for both autocatalytic reactions and polymerization.

## *Integrating Design and Control by Embedded Control Optimization Method*

Friday, October 1, 2010: 1:30 PM

Armour Dining (Illinois Institute of Technology)

Andreas A. Linninger, Laboratory for Product and Process Design, University of Illinois at Chicago, Chicago, IL

For last 30 years, chemical process researchers devoted to integrating design and control, in which the design decisions, dynamics, and control performance are considered simultaneously in the optimal fashion. Rigorous incorporation of the process dynamics is important for operational safety and efficiency and may lead better overall system performance. However, rigorous methods for solving design and control simultaneously lead to challenging mathematical formulations which easily become computationally intractable. Our Embedded Control Optimization method reduces nonlinear dynamic combinatorial complexity into linear state space model and achieves a tractable mathematical programming formulation. Further, we extended our methodology to large-scale plantwide processes which have the large computational time requirement making it impossible to apply current optimization algorithms. The case study that is plantwide scale isomerization flowsheet demonstrates the capability of our method for the control and design integration in a large scale flowsheet.

## *Modeling of Biochemical Reactors – Role In Analysis, Design, Optimization and Control*

**Friday, October 1, 2010: 2:00 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Satish J. Parulekar, Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, IL

Biochemical reactors involve use of biocatalysts (enzymes) in the absence or presence of life. Biological catalysts used outside living cells include extracellular enzymes and immobilized enzymes. A living cell is a complex chemical reactor in which a large number of independent reactions, catalyzed by intracellular enzymes, occur. Each individual cell is a complicated multi-component system subject to a complex set of internal controls. The cellular environment is very often a multiphase system comprised of gas, liquid and solid phases and the nutrient medium used for cell cultivation is as a rule a multi-component mixture. External controls may regulate some of the environmental parameters. All of these can influence cell kinetics significantly. Depending on their intended use, whether it be obtaining a detailed and fundamental insight into metabolism of living cells, design and optimization of bioreactors and fixing operational protocols for these, or precise control of operation of these, kinetic models with different levels of sophistication have been developed and used. An overview of mathematical models for biochemical reactors will be provided and their utility in analysis, design, optimization and control of bioprocesses will be illustrated.

## *New Trends In Monitoring and Supervision of Distributed Processes: Towards Fault-Tolerant Control*

**Friday, October 1, 2010: 2:30 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Ali Cinar, Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, IL

Software environments that enable the use of competing techniques for process monitoring and fault diagnosis will be presented and an adaptive process supervision system that can change confidence in monitoring and diagnosis results based on past experience will be introduced. The linkage between such software and control systems will be discussed to develop a fault-tolerant control environment by using distributed intelligence.

## *Industrial Applications of Rule-Based Systems*

**Friday, October 1, 2010: 3:00 PM**

[Armour Dining \(Illinois Institute of Technology\)](#)

Jeffrey D. DeCicco and Douglas Myers, Intelligent Laboratory Solutions, Warrenville, IL

Rule-based systems have found application in industrial process monitoring and control. Most often the application of real-time rules complements model based approaches. ILS will provide industrial applications of rule-based system for process control and monitoring for biotech applications, oil and chemical, and energy applications.

# Renewable Energy

Friday, October 1, 2010: 1:00 PM  
Trustee Room (Illinois Institute of Technology)

## Description:

The key challenges in establishing a sustainable biomass infrastructure are the following: • Sustainable feedstock supply chain • Development of efficient feedstock flexible process technologies • Production of fungible fuels that can leverage existing transport and fuel infrastructure • Product qualities that are at par or better than their fossil counterparts • Overall economics that make drive substitution without the need for government subsidies • Demonstrated life cycle emission benefits over its fossil counterparts This session will provide an overview of the various feedstock and technology options, project investment drivers, and a discussion of Life cycle analyses for biofuels derived from a variety of feedstocks.

## Chair:

Prabhakar Nair

Email: [Prabhakar.Nair@uop.com](mailto:Prabhakar.Nair@uop.com)

## *Biofuels and BioEnergy Overview*

Friday, October 1, 2010: 1:00 PM

[Trustee Room \(Illinois Institute of Technology\)](#)

Stanley Frey, Aromatics and Derivatives Development, UOP LLC, Des Plaines, IL

Global primary energy demand over the next two decades will increase by almost 50 percent. To meet this future demand all forms of energy will need to be tapped, conventional as well as unconventional. In the unconventional category, renewable energy will play an increasingly important role in the future primary energy mix. The growth of renewable energy is driven primarily by government legislation and tax incentives that promote this form of energy. Renewable energy, if sustainably produced, can also help combat global warming trends. This presentation will cover some of the key energy trends, and also provide an overview of the renewable technology solutions that UOP has developed for commercial application in both the transport fuel and heat & power segments.

## *Pennycress: a Sustainable Energy Crop for Biofuels Production*

Friday, October 1, 2010: 1:25 PM

[Trustee Room \(Illinois Institute of Technology\)](#)

Peter B. Johnsen, Arvens Technology Inc., Peoria, IL

Arvens Technology Inc. (ATI) is developing Field Pennycress (*Thlaspi arvense* L.) as a sustainable, low impact energy crop for biofuels production with unique economic, environmental and social benefits.. Pennycress yields more than 2000 pounds per acre of seeds that contain 36% oil with a composition that is suitable for conversion to biodiesel while requiring few inputs. It is non-food member of the mustard family grown as a winter annual planted after the fall corn harvest and harvested before planting soybeans in the spring on land that is otherwise left bare over the winter. This avoids the food vs fuel and indirect land use issues completely. The ATI strategy is to develop Pennycress in the upper Mid-west corn-belt where approximately 40 million acres planned for soybeans are left bare and unused during the winter each year. ATI and its USDA research partners have produced FAME biodiesel meeting ASTM 6751 standards from unrefined seed oil and utilized fast pyrolysis to produce a uniquely stable bio-oil from the de-oiled presscake. The presentation will cover agronomic and processing research underway to commercialize Pennycress as a dedicated energy crop.

## *Syngas to Ethanol*

**Friday, October 1, 2010: 1:50 PM**  
Trustee Room (Illinois Institute of Technology)  
Steve Donnellan, Coskata, Warrenville, IL

Mr. Steve Donnellan will provide an overview of Coskata's three-step syngas-to-ethanol process, and the platform's readiness to deploy cellulosic ethanol technology at a commercial scale. Following the successful unveiling and operation of Coskata's semi-scale demonstration facility in Madison, Pennsylvania, Coskata has proven the commercial viability of the syngas-to-ethanol platform and the value that gasification technology brings to ethanol production all in one integrated process. Donnellan can elaborate on the benefits of the syngas-to-ethanol platform, which is one the most affordable, efficient, flexible, and sustainable ways to produce cellulosic ethanol in the mandated renewable fuels market. He will elaborate on the efficiency of the platform, illustrating its ability to be price-competitive with oil, yielding more than 100 gallons per dry ton of input material.

## *Integrated Bio-Refinery Automation Solutions*

**Friday, October 1, 2010: 2:15 PM**  
Trustee Room (Illinois Institute of Technology)  
Ganesh Venimadhavan, Honeywell Process Solutions, Carmel, IL

Renewable fuels have become a very important part of the fuel mix especially in OECD countries. Because of the bulky nature of the renewable feedstock, unlike conventional refining, renewable fuel processing units has to be distributed. In addition, in many cases, the operators of renewable fuel processing units may not have the resources and/or the extensive experience in running process units. One solution to this problem is a packaged process plant which includes process automation including appropriate sensors and other field devices, regulatory control (DCS), safety systems, graphics, advanced process control and automated checklists for procedures both for standard tasks and for infrequent tasks such as startups and shutdowns with the process design. The packaged plant approach would help reduce start-up time, ensure safe and consistent operations and maximize processing capacity and/or minimize energy consumption subject to the constraints of the unit. It would also reduce the burden and the risk for the unit operator by having a one stop shop for both the process and automation needs. It would also provide a single accountable entity that would resolve/fix any problems going forward.

## YPAB – Sessions

### *Young Professionals Workshop - Résumé Workshop*

**Thursday, September 30, 2010: 12:30 PM**  
Armour Conference (Illinois Institute of Technology)

**Description:**

With increased competition in today's job search market, you have to be sure your résumé stands out in the crowd. Work one-on-one with a local Young Professional and learn strategies to fine tune your résumé.

**Chair:**

Jessica Swary

**Email:** [Swaryjr@Middough.com](mailto:Swaryjr@Middough.com)

### *Young Professionals Workshop - to FE or Not to FE*

**Thursday, September 30, 2010: 3:00 PM**  
Armour Conference (Illinois Institute of Technology)

**Description:**

Still deciding to whether or not to take the FE Exam? Not sure if you really need a PE license as a ChemE? Come meet our panel of active Chemical Engineer Professional Engineers and hear first-hand why you need it and what it takes. Impending changes to licensure requirements will also be discussed.

**Chair:**

Bill Glogowski

**Email:** [Glogowwk@Middough.com](mailto:Glogowwk@Middough.com)

### *Innomag Pump Demonstration*

**Thursday, September 30, 2010: 12:30 PM**  
Trustee Room (Illinois Institute of Technology)

**Description:**

Professional Matthew Moy from INNOMAG in Addison, IL will lead an interactive demonstration on sealless non-metallic magnetically driven pumps.

**Chair:**

Jessica Swary

**Email:** [Swaryjr@Middough.com](mailto:Swaryjr@Middough.com)

**Co-Chair:**

Matthew Moy

**Email:** [moymatt@gmail.com](mailto:moymatt@gmail.com)

## *Improvisation for Engineering Innovation*

**Friday, October 1, 2010: 9:30 AM**  
Ballroom (Illinois Institute of Technology)

### **Description:**

Enhanced creativity among U.S. engineers and scientists is required in the face of strategic needs for innovation in numerous technical areas including: energy, the environment and health. NSF's third generation Engineering Research Centers explicitly require an educational component to enhance creativity to improve innovation. We have applied an approach to improving creativity that has traditionally not been used in technical innovation. The approach uses improvisational humor exercises to generate innovative ideas. The equivalence of humor and innovation is well established, and recently Sweeney and co-workers have systematically applied improvisation to enhance innovation. While this approach has been successful in non-technical fields, such as business and marketing, success has been limited in technical fields such as engineering. We have suggested a protocol based on a combination of humorous improvisation and stochastic molecular simulation to effectively search technical idea space. Humorous improvisation is the random idea generator for a stochastic search algorithm in innovation space; just as random number generators are used to sample molecular conformation space. We hypothesize that a more comprehensive refinement of idea space is required to make this approach effective for technical innovation. We have made some preliminary investigations of this protocol by carrying out workshops with undergraduate engineering design students. These preliminary results have suggested a basic protocol that uses a two-stage process: an improvised random idea which then inspires a technical problem solution. This two step approach is not used in Sweeney's approach, and may be responsible for its lack of effectiveness in technical areas.

### **Chair:**

Jessica Swary

**Email:** [Swaryjr@Middough.com](mailto:Swaryjr@Middough.com)

### **Co-Chair:**

Daniel Archer

**Email:** [darche3@uic.edu](mailto:darche3@uic.edu)

## *Young Professionals Workshop - Mock Interviews*

**Friday, October 1, 2010: 1:00 PM**  
Armour Conference (Illinois Institute of Technology)

### **Description:**

Whether you are looking for your first internship or full-time position, the interview is your chance to sell yourself and make a great first impression. As with most things, practice makes perfect. Come practice your interview skills with local Young Professionals and learn tips and tricks to help you land that perfect position

### **Chair:**

Bill Glogowski

**Email:** [Glogowwk@middough.com](mailto:Glogowwk@middough.com)

# 2010 AIChE Midwest Regional Conference

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Session Chair: Jeff Kitz, Middough, Inc	Title: Process Industry Practices
Session Chair: Kevin Taylor	Title: Energy and the Environment
Session Chair: Pete Ludovice	Title: Humor in Engineering Innovation
Session Chair: Justin Notestein, NU	Title: NU Recent Research Results
Session Chair: Urmila Diwekar, VRI-CUSTOM	Title: Sustainable Energy Systems
Session Chair: Prabhakar Nair, UOP	Title: UOP Renewable Chemicals Developments

**YPAB Sessions:**

Session Chair: Jessica Swary, Middough	Title: Resume Workshop
Session Chair: Bill Glogowski, Middough	Title: Mock Interview / To FE or not to FE

### HS Outreach Program:

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# 2011 AIChE Spring Meeting & 7<sup>th</sup> Global Congress on Process Safety

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# Save the Date



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