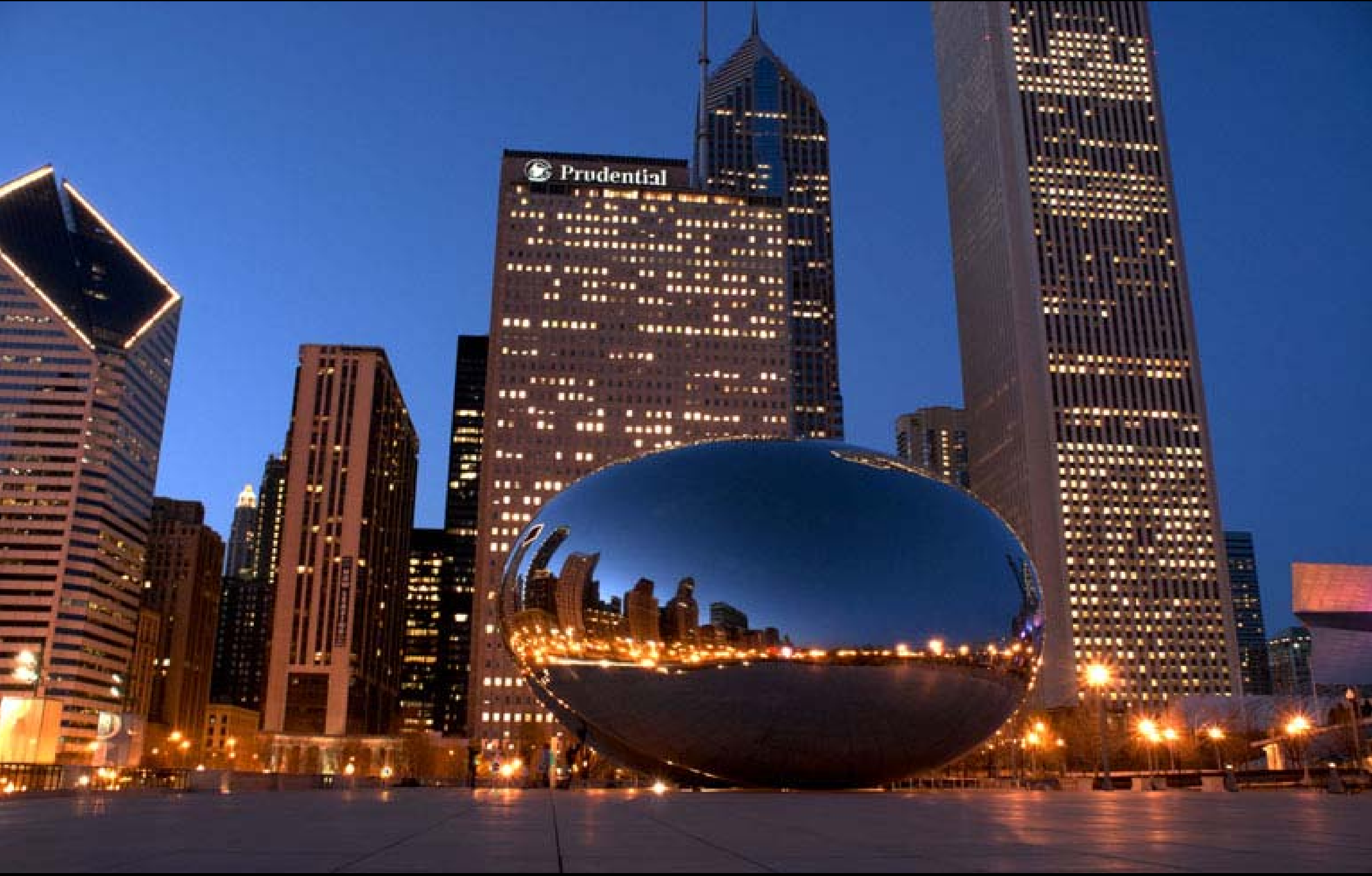

2009 AIChE
Midwest Regional Conference
Chicago, IL October 5-6, 2009

Addressing Current Critical Issues – Energy & Sustainability

The Chicago Local Section of the
American Institute of Chemical Engineers

University of Illinois at Chicago

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Introduction

Building on last year's successful Midwest Regional conference, the Chicago Local Section, along with AIChE National and IEEE support, is continuing its programming efforts to provide an opportunity to engineers and scientists in the region to learn about new technologies, as well as offer a relaxed setting for networking. This year's conference focuses on the critical subjects of **energy and sustainability**.

Plus, the Chicago Local Section, along with the University of Illinois at Chicago, is pleased to continue sponsoring the **High School Engineering Career Outreach Program**. Chicago-area high school students will become acquainted with the various facets of the chemical engineering profession. The program will take place on both days from 10:00am – 1:00pm, and the featured speaker is former NASA payload specialist and current professor of chemical engineering at Northeastern University, **Dr. Al Sacco**. The program includes a special luncheon where students can interact with practicing chemical engineers. For young professional engineers, a workshop will be held on both days to help fine-tune interviewing skills and improve the effectiveness of resumes.

Other highlights include:

- Opening Remarks for Symposium: **Dr. Reza Mostofi-Ashtiani,** UOP LLC and Chair, Chicago Section AIChE, and **Dr. Sohail Murad,** Professor and Head of the Department of Chemical Engineering, UIC
- Monday Keynote Speaker: **Walter W. Kovalick, Jr., Ph.D.,** Assistant Regional Administrator for Resources Management, U.S. EPA
- Tuesday Keynote Speaker: **Guenter Conzelmann**, Director of the Center for Energy, Environmental, and Economic Systems Analysis (CEEESA), Argonne National Laboratory
- A monthly meeting for the AIChE Chicago Section will be held on Monday evening, with guest speaker **Marcus Tennant,** Principal Systems Architect, Yokogawa Corp. of America

Please look at the inside front cover of this program book as well as our website, http://www.aiche.org/Conferences/2009chicagoconference.aspx, to see the many corporate sponsors who helped to make this program possible, both through financial assistance and the time its staff spent helping and attending the programs.

Welcome, from the 2009 Symposium Organizing Committee.

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Program Grid: Special Events

Time	Description	Location
Monday 8:15 - 8:30AM	**Welcoming Remarks**	Illinois A/B
	Dr. Reza Mostofi-Ashtiani, UOP LLC and Chair of Chicago Section AIChE; Dr. Sohail Murad, Professor and Head of the Department of Chemical Engineering, UIC	
Monday 8:30 - 9:20AM	**Monday Keynote Address**	Illinois A/B
	Energy, Climate Change and Sustainability Walter (Walt) W. Kovalick, Jr., Ph.D., Assistant Regional Administrator for Resources Management, United States Environmental Protection Agency	
Monday & Tuesday 10:00 AM – 1:00PM	**High School & Community Outreach Program** (see page 12 for more information)	Illinois A/B
Monday 1:30 – 3:30 PM	**AIChE Midwest Regional Resume Workshop** **(sponsored by the Young Professionals Advisory Board)**	White Oak A/B
	Freshen up your résumé with one-on-one help from local Young Professionals. Make sure to bring your résumé!	
Monday 6:00 – 8:30 PM	**Chicago Local Section Dinner**	Illinois A/B
	Enjoy dinner with your fellow chemical engineers. Hear Marcus Tennant, Principal Systems Architect for Yokogawa Corp. of America, discuss “Automation of Batch and Procedural Control.” Also, Harold H. Kung will be presented with the Thiele Award.	
Tuesday 8:30 - 9:20AM	**Tuesday Keynote Address**	Illinois A/B
	Sustainability and the Case for Transformational Research Guenter Conzelmann, Director of the Center for Energy, Environmental, and Economic Systems Analysis (CEEESA), Argonne National Laboratory	
Tuesday 1:30 – 3:30 PM	**AIChE Midwest Regional Interview Workshop** **(sponsored by the Young Professionals Advisory Board)**	White Oak A/B
	Practice your interview skills with one-on-one help from local Young Professionals.	
Tuesday 5:30 – 8:00 PM	**AIChE Young Professionals Happy Hour Mixer**	Spectrum Bar & Grill, 233 S. Halsted
	Come and meet other local students and AIChE Young Professionals. Appetizers and soda will be provided.	

Program Grid: Technical Sessions - Monday, October 5, 2009

Welcoming Remarks and Keynote Presentation		**Location: Illinois A/B**
Time	**Presentation Title**	**Speaker(s)**
8:15 - 8:30 AM	Welcoming Remarks	Dr. Reza Mostofi-Ashtiani, UOP LLC and Chair of Chicago Section AIChE; Dr. Sohail Murad, Professor and Head of the Department of Chemical Engineering, UIC
8:30 - 9:20 AM	Keynote – Energy, Climate Change and Sustainability	Walter (Walt) W. Kovalick, Jr., Ph.D., Assistant Regional Administrator for Resources Management, United States Environmental Protection Agency

Illinois Institute of Technology Research on Energy & Sustainability		**Location: Cardinal**
Time	**Presentation Title**	**Speaker(s)**
9:30 - 10:05 AM	Numerical Simulation of Fluid-Multi- Type Particle Flow System	Hamid Arastoopour and Matteo Strumendo Department of Chemical and Biological Engineering, IIT
10:05 - 10:40 AM	Profit Control: A New Approach to Control System Design	Donald J Chmilelewski and Benjamin Omell Department of Chemical and Biological Engineering, IIT
10:40 - 11:15 AM	The Emerald Forest: An Integrated Approach to Bioenergy and Sustainable Communities	Fouad Teymour Department of Chemical and Biological Engineering, IIT
11:15 - 11:50 PM	Smart Grid: A New Paradigm of Power Delivery	Mohammad Shahidehpour Department of Electrical and Computer Engineering, IIT

Engineering Opportunities in Sustainable Development		**Location: Tower 713**
Time	**Presentation Title**	**Speaker(s)**
9:30 AM– 12:00 PM	Overview of Sustainable Development Challenges	Jim Van der Kloot, U.S. Environmental Protection Agency
	Green Stormwater Management Practices	Bob Newport, U.S. Environmental Protection Agency
	Green Streets and Alleys	Janet Attarian, Chicago Dept of Transportation
	Panel Discussion	Moderated by Dennis O'Brien, Jacobs Consultancy

Program Grid: Technical Sessions - Monday, October 5, 2009

Solar Cells and Thermoelectrics		Location: Tower 613
Time	**Presentation Title**	**Speaker(s)**
9:30 AM – 12:00 PM	Solar Cells Based on CdTe Thin Film and Composite of Organic and Inorganic Nano-scale Materials	Ms. Hyeson Jung, University of Illinois at Chicago
	Energy Harvesting Using Piezoelectric Materials – A Review	Dr. Banani Sen and Dr. Mitra Dutta, University of Illinois at Chicago
	Analysis of the Fundamental Structure-Property Relationships in Thermoelectric $Ca_3Co_4O_9$	Professor Robert Klie, University of Illinois at Chicago

University of Illinois at Urbana-Champaign (UIUC) Research on Sustainable Energy		Location: Cardinal
Time	**Presentation Title**	**Speaker(s)**
1:00 – 5:00 PM	Reconstitution of an Enzyme Mixture from the Fiber Degrading Rumen Bacterium, Prevotella bryantii B_14 which is Capable of Deconstructing Hemicellulose	Dylan Dodd, Shinichi Kiyonari, Yejun Han, Charles M. Schroeder, Roderick I. Mackie, Isaac K. O. Cann, UIUC
	Recombinant Yeast Strains Towards Consolidated Bioprocessing: Surface Display of Functional Mini-cellulosomes for Direct Conversion of Cellulose to Ethanol	Fei Wen, Jie Sun, and Huimin Zhao, UIUC
	Engineering an L-arabinose/xylose Co-utilizing S. cerevisiae for Biofuels Production	Tae-Hee Lee and Huimin Zhao, UIUC
	Microbial Synthesis of Xylitol from Hemicellulose	Ryan Sullivan and Huimin Zhao, UIUC
	Electrode Characterization Using an Alkaline Microfluidic H_2/O_2 Fuel Cell as an Analytical Platform	Matt S. Naughton, Fikile R. Brushett, and Paul J. A. Kenis, UIUC

Program Grid: Technical Sessions - Monday, October 5, 2009

Perspectives on Energy and Sustainability		**Location: Tower 713**
Time	**Presentation Title**	**Speaker(s)**
1:00 – 5:00 PM	The Energy and Sustainability Challenges	George Crabtree, Argonne National Laboratory
	Chicago's Vision for Energy and Sustainability	David O'Donnell and Dana Kenney, Department of the Environment, City of Chicago
	The Initiative for Sustainability and Energy at Northwestern University	David C. Dunand, Northwestern University
	Sustainability in the Urban University	Cynthia (Cindy) Klein-Banai, University of Illinois at Chicago
	The Business of Sustainability: *The balance between profit and progress…*	Peter Dreiske, EPIR Technologies, Inc.

Future Electrical Energy Generation and Distribution		**Location: Tower 613**
Time	**Presentation Title**	**Speaker(s)**
1:00 – 5:00 PM	The Potential of Smart Grid in Illinois	Jim Crane, ComEd
	Wind Forecasting and Integration into Power System Operations	Jianhui Wang, Argonne National Laboratory
	Minimization of Water Consumption Under Uncertainty for Pulverized Coal (PC) Process	Juan M. Salazar and Urmila M. Diwekar, Vishwamitra Research Institute: Center for Uncertain Systems Tools for Optimization and Management and Collaboratory for Process & Dynamic Systems Research, National Energy Technology Laboratory
	Stochastic Modeling of Biodiesel Production Process	Sheraz Abbasi and Urmila Diwekar, University of Illinois -Chicago

Program Grid: Technical Sessions - Tuesday, October 6, 2009

Keynote Presentation		**Location: Illinois A/B**
Time	**Presentation Title**	**Speaker(s)**
8:30 - 9:20 AM	Sustainability and the Case for Transformational Research	Guenter Conzelmann, Director of the Center for Energy, Environmental, and Economic Systems Analysis (CEEESA), Argonne National Laboratory

Biomass Energy		**Location: Cardinal**
Time	**Presentation Title**	**Speaker(s)**
9:30 AM – 12:00 PM	Biomass Gasification	Michael Roberts, Gas Technology Institute
	Glass-Ceramic Catalysts for Tar Decomposition in Biomass Gasification	Logan Weast, Gas Technology Institute
	Integrated Hydropyrolysis and Hydroconversion Process for Production of Gasoline and Diesel Fuel from Biomass	Terry Marker, Larry Felix and *Martin Linck,* Gas Technology Institute
	Biogas Cleanup and Use	Ted Barnes, P.E., Gas Technology Institute

Medical Imaging Advances		**Location: Tower 613**
Time	**Presentation Title**	**Speaker(s)**
9:30 AM – 12:00 PM	Development of a Magnetic Resonance Diffusion Tensor Template of the Human Brain	Konstantinos Arfanakis, BME Department, IIT
	Automated Image Diagnostic-Quality Characterization	Jovan Brankov, ECE Department, IIT
	Phase-Contrast Imaging and the Potential for Low-Dose Mammography	Adam Zysk, ECE Department, IIT
	Limited Data Image Reconstruction in Photoacoustic Tomography	Kun Wang, BME Department, IIT

Program Grid: Technical Sessions - Tuesday, October 6, 2009

Catalysis for Energy		**Location: Tower 713**
Time	**Presentation Title**	**Speaker(s)**
9:30 AM – 12:00 PM	Energy Efficient Catalysts and Processes for the Petrochemical Industry: Future Challenges in Energy	Javier Guzman, Mike Bedell, and Bruce R. Cook, BP North America
	Kinetic Monte Carlo Simulation for $(\sqrt{5}x\sqrt{5})R27°$ Surface Oxide over Pd(100)	Jelena Jelic, Randall Meyer, University of Illinois at Chicago Karsten Reuter, Fritz Haber Institute
	In-situ XAFS analysis for the synthesis and testing of supported Pt catalysts for propane oxidation	Worajit Setthapun[1], Jeffrey W. Elam[1], Federico A. Rabuffetti[2], James A. Enterkin[2], Kenneth R. Poeppelmeier[2], Laurence D. Marks[2], Peter C. Stair[1,2], Jeffrey T. Miller[1], and Christopher L. Marshall[1] [1]Argonne National Laboratory; [2]Northwestern University
	Selective Adsorption of Manganese onto Cobalt for Optimized $Mn/Co/TiO_2$ Fischer-Tropsch Catalysts	Theresa Feltes[1], Randall Meyer[1], Bert Weckhuysen[2], John Regalbuto[1] [1]University of Illinois at Chicago; [2]Utrecht University
	Glycosidic Bond Cleavage in Oxidative Hydrolysis of Cellulosic Materials	Weiling Deng, Sungsik Lee, Stefan Vajda, Joseph A. Libera, Jeffrey W. Elam, and Christopher L. Marshall, Argonne National Laboratory
	Catalysis for the Generation of Biofuels	William C Ketchie and Joseph A. Kocal, UOP LLC – A Honeywell Company

Program Grid: Technical Sessions - Tuesday, October 6, 2009

Alternative Fuels		Location: Cardinal
Time	**Presentation Title**	**Speaker(s)**
1:00 – 5:00 PM	Inhibition of the Switch from Glucose to Xylose by Ethanol Concentration: The Advantage of the Cell Recycle	P.J. Slininger, National Center for Agricultural Utilization Research, USDA-ARS
	Biomass fuel for Combined Heat and Power	Dean Karafa, Middough
	GLBRC Thrust 2 Efforts to Deconstruction Plant Cell Wall to Fermentable Sugars and Fuel Molecules	Venkatesh Balan and Bruce Dale, Michigan State University
	Enzymes Screening and Optimization for Hydrolysis On Ammonia Fiber Expansion Treated Corn Stover	Dahai Gao, Shishir P. S. Chundawat, Bruce E. Dale and Venkatesh Balan, Michigan State University
	Ultra-structural and Physicochemical Modifications within Ammonia Pretreated Lignocellulosic Cell Walls that Influence Enzyme Accessibility	Leonardo da Costa Sousa[1], Shishir P. S. Chundawat[1], Bryon S. Donohoe[2], Lekh Sharma[3], Thomas Elder[4], Per Askeland[1], Ramin Vismeh[1], Umesh Agarwal[5], James Humpula[1], Rebecca Garlock[1], Daniel A. Jones[1], Kevin Chambliss[3], Michael E. Himmel[2], Balan Venkatesh[1], Bruce E. Dale[1]. [1]Michigan State University; [2]National Renewable Energy Laboratory; [3]Baylor University; [4]USDA-Forest Service, Southern Research Station; [5]USDA-Forest Products Laboratory

Solid State Lighting and Sensors		Location: Tower 613
Time	**Presentation Title**	**Speaker(s)**
1:00 – 5:00 PM	Brightness and Wavelength Dependence of Blue LEDs Upon Sapphire Off-cut Angle and Sapphire Patterning	Dr. Heinz Busta, Prairie Prototypes, LLC and University of Illinois at Chicago
	Infrared Detectors	Mr. Koushik Banerjee, University of Illinois at Chicago
	Confined Phonon Modes and Thermal Conductivity in Graphene	Mr. Jun Qian, University of Illinois at Chicago

Program Grid: Technical Sessions - Tuesday, October 6, 2009

Novel Materials and Processing for Energy & Sustainability		**Location: Tower 713**
Time	**Presentation Title**	**Speaker(s)**
1:00 – 5:00 PM	Next Generation of Rechargeable Li-ion Batteries: Challenges, Opportunities, and Advances at Northwestern	Jung-Kyoo Lee, Kurt Smith, Cary Hayner, and Harold Kung*, Northwestern University
	Development of Nanostructured Thermoelectric Materials for More Efficient Heat-to-Power Generation	Steven N. Girard and Mercouri G. Kanatzidis, Northwestern University
	Titania Thin Films Prepared by Reactive Sputtering: Non-Stoichiometry and Cation Doping	Paul Desario, Le Chen, Michael Graham, Kimberly Gray, Northwestern University
	Advances in Synergistic Polymer/Graphite and Polymer/Carbon Nanotube Nanocomposites and Sustainable Polymer Systems Using a Novel, Industrially Scalable Process Called Solid-State Shear Pulverization	John Torkelson,* Jun'ichi Masuda, Katsuyuki Wakabayashi, Cynthia Pierre, and Philip Brunner, Northwestern University
	Novel Green Light Emitting Diodes: Innovative Droop-free Lighting Solutions for a Sustainable Earth	C. Bayram,[a] F. Hosseini Teherani,[b,] D. J. Rogers,[b] R. McClintock,[a] and M. Razeghi*[a] [a] Northwestern University; [b]Nanovation SARL
	Separations of CO_2/CH_4 and CO_2/N_2 Mixtures Using Metal-Organic Frameworks	Youn-Sang Bae, Omar K. Farha, Karen L. Mulfort, Alexander M. Spokoyny, Chad A. Mirkin, Joseph T. Hupp, and Randall Q. Snurr, Northwestern University

The American Institute of Chemical Engineers
And The University of Illinois Chicago
WELCOMES HIGH SCHOOL &
COMMUNITY COLLEGE STUDENTS
October 5 and 6, 2009

Being an Engineer—Creating A World That Works!

10:00 AM **WELCOME AND OPENING COMMENTS**
Alan Zagoria, Chemical Engineer, UOP

10:05 AM **ENGINEERING TO CHANGE THE WORLD**
Panel of invited chemical engineering students

10:35 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.

11:30 AM **THE ENGINEERING EXPERIENCE: A PANEL DISCUSSION**
Rick Isherwood, UOP

12:00 PM **HS COMPETITION: WHAT KIND OF ENGINEER AM I?**
Emceed by Alan Zagoria, Chemical Engineer, UOP
Participants: Selected HS Student Representatives

12:15 PM **LUNCH & CHAT WITH PROFESSIONAL ENGINEERS**
A time for personal conversation with real engineers
Hosted by UIC and the AIChE Chicago Section

KEYNOTE PRESENTATIONS

Monday, October 5, 2009 – 8:30 – 9:20 AM

Energy, Climate Change and Sustainability

Walter (Walt) W. Kovalick, Jr., Ph.D., Assistant Regional Administrator for Resources Management, United States Environmental Protection Agency

Biography

Dr. Kovalick acts as the senior official for management and administration for EPA's Regional Office in Chicago, which works jointly with states and tribes in the six Midwestern states—Illinois, Indiana, Ohio, Michigan, Wisconsin, and Minnesota to carry out EPA's environmental protection mission. For this 1,200 person organization, his responsibilities encompass human resources, information technology, geographic information support, facilities, budget, and contracts and grants. He is the senior resource official accountable for the region's $700M budget, which includes over $540M in contracts and grants.

Dr. Kovalick holds a Bachelor of Science in Industrial Engineering and Management Science from Northwestern University and a Masters in Business Administration from Harvard Business School. He holds a Ph.D. in Public Administration and Policy from Virginia Polytechnic Institute. He is twice a recipient of the President's Meritorious Executive Award, as well as EPA Bronze and Silver Medals for Superior Service. In February, 1991, he was named by Engineering News-Record magazine as one of their "1990 Marksmen." In 1997, he received the EPA Fitzhugh Green Award for Outstanding Contributions to International Environmental Protection over 20 years. In May 2000, he received the Virginia Tech College of Architecture and Urban Studies Alumni Award for Outstanding Professional Accomplishment. In June 2000, he received an EPA Manager's Award for Diversity for his work on minority recruitment.

Tuesday, September 23, 2008 – 8:30 – 9:20 AM

Sustainability and the Case for Transformational Research

Guenter Conzelmann, Director of the Center for Energy, Environmental, and Economic Systems Analysis (CEEESA), Argonne National Laboratory

Biography

Mr. Guenter Conzelmann is the Director of the Center for Energy, Environmental, and Economic Systems Analysis at Argonne National Laboratory. His center develops new modeling and simulation tools and provides analytical services to government institutions and private sector clients around the world on strategic energy and environmental issues. In recent years, Mr. Conzelmann has focused his interests on applying complex systems theories and agent-based modeling approaches to short and long-term simulations of energy markets, including restructured power markets, and the evolution of new transportation infrastructures.

Mr. Conzelmann is Argonne's program lead for wind and solar integration issues and also leads Argonne's building technologies activities. He is the author/co-author of numerous publications, including sponsor reports, conference papers, journal articles, and book contributions in the energy and environmental field. He is frequently invited to speak on these subjects at conferences, workshops, and training courses around the world.

Illinois Institute of Technology (IIT) Research on Energy and Sustainability

Chair: Don Chmielewski, IIT

Monday, October 5, 9:30-10:05am

Numerical Simulation of Fluid-Multi- Type Particle Flow System

Hamid Arastoopour and Matteo Strumendo
Department of Chemical and Biological Engineering, IIT

The kinetic theory for granular flow was extended to mixtures of multi-type particles assuming a non-Maxwellian velocity distribution and energy non-equipartition. Each type of particle was considered as a separate phase with different velocity and granular temperature. The resulting momentum equation for each particulate phase includes phase interaction arising from collision pressure and particle-particle drag force. This model was applied to study flow of multi-type particles (incorporated in the MFIX Code) in the riser section of the circulating fluidized bed systems.

To account for continuous variation in particle size and density distribution due to phenomena such as reaction, agglomeration, nucleation and growth at significantly less required computational time, a new approach to solve PBE (Population Balance Equations), FCMOM (Finite size domain Complete set of trial functions Method of Moments) is presented. The solution of the PBE is sought, instead of the $[0,\infty]$ range in the finite interval between the minimum and maximum particle size; their evolution is tracked imposing moving boundaries conditions. After reformulating the PBE in the standard interval $[-1,1]$, the size distribution function is presented as a series expansion by a complete system of orthonormal functions. Moments Evolution Equations are developed from the PBE in the interval $[-1,1]$. The FCMOM is implemented through an efficient algorithm and provides the solution of the PBE both in terms of the moments and in terms of the size distribution function. The FCMOM was validated with applications to particle growth, nucleation, particle aggregation, and linked with flow equations (CFD) to solve non-homogeneous flow system in a riser, and crystallization processes.

Monday, October 5, 10:05-10:40 am

Profit Control: A New Approach to Control System Design

Donald J Chmilelewski and Benjamin Omell
Department of Chemical and Biological Engineering, IIT

Since the inception of feedback, there has been a strong, but vague, relationship between control system performance and plant profit. This presentation will highlight recent efforts to quantify such a relationship so as to arrive at controller designs tailored not only to the dynamics of the plant but also to the specific economic situation. A powerful tool for the economic analysis of dynamic systems is that of Backed-off Operating Point Selection (BOPS). In general, the BOPS approach is to calculate an Expected Dynamic Operating Region (EDOR) and optimize its location within a given constraint set. However, if the controller is re-tuned, then the shape of the EDOR will change and result is a new BOPS. Thus, simultaneous optimization over controller parameters and the EDOR location will yield not only greater profit but also controller that is tuned to exploit its economic and constraint environment. The procedure will be illustrated by a number of application studies, ranging from reactor and inventory control systems to simultaneous system/controller design for hybrid fuel cell vehicles.

Monday, October 5, 10:40-11:15 am

The Emerald Forest: An Integrated Approach to Bioenergy and Sustainable Communities

Fouad Teymour
Department of Chemical and Biological Engineering, IIT

The Emerald Forest is a vision aiming at displacing a significant portion of the US and worldwide consumption of fossil fuels for energy needs, and at reclaiming vast areas of arid and desert land for sustainable community development. The concept addresses three major crises of national and worldwide proportions and proposes an integrated approach towards the alleviation of their impact on the quality of life for humankind. These deal chiefly with the energy crisis, the climate change and loss of green mass challenges, and the global need for affordable shelter and housing.

The approach centers on the massive-scale production of aquatic algal biomass without the use of fresh water or arable land. It couples the biomass production with the development of sustainable communities, through the reclamation of arid and/or uninhabitable regions, in order to improve the economics of the required capital expenditure. At the core of the proposed vision are massive artificial forests, to be created in desert lands that are in proximity of ocean waters. Many such areas are available in the United States and worldwide. This approach relies on vertical integration and massive scale design to provide a global sustainable solution. The forest consists

of tree-like bioreactors filled with seawater and algae and continuously fed with carbon dioxide and nutrients. The tree-like design is selected for its natural efficiency in capturing sunlight.

The presentation introduces the concept, explains the reasoning behind the integrated approach, and discusses all the technical challenges that need to be resolved to bring it to realization. It also focuses on the detailed analysis of one of the specific challenges, namely the design of an optimized optical assembly for efficient collection and distribution of sunlight to the bioreactor interiors. The utilization of FLUENT simulations using the Radiative Transfer Equation (RTE) approach is presented, along with simulation results for a number of simple and compound waveguides and light distribution elements.

Monday, October 5, 11:15-11:50 am

Smart Grid: A New Paradigm of Power Delivery

Mohammad Shahidehpour
Department of Electrical and Computer Engineering, IIT

This presentation will highlight some of the key issues in the smart grid design and applications. Smart grid represents a vision for a digital upgrade of electric power transmission and distribution. It optimizes the grid operations, enhances the grid security, and opens up new markets for the utilization of sustainable energy production. Smart grid is an aggregate term for a set of related technologies for electric power systems rather than a name for a specific technology with a generally agreed on specification. The key to a smart grid is using the Internet protocol on home devices to shuttle information back and forth between the electric utility and customers. A smart meter installed at consumer premise measures, monitors, and helps manage how much energy is used. With a smart two-way communications mechanism between a power consumer and its provider, both parties can get far more control over electric power consumption, cost, outages, and security.

The development of a prototype model of smart grid which is funded by the U.S. Department of Energy and being implemented at the Illinois Institute of Technology will be discussed. The global IEEE activities for promoting smart grid technologies will also be discussed. At the end of the presentation, a short video on smart grid, which is produced by the IEEE Power and Energy Society, will be exhibited.

Engineering Opportunities in Sustainable Development

Chair: James Van der Kloot, U.S. Environmental Protection Agency

Monday, October 5, 9:30am – 12:00pm

Overview of Sustainable Development Challenges
James Van der Kloot
U.S. Environmental Protection Agency

Green Stormwater Management Practices
Bob Newport
U.S. Environmental Protection Agency

Green Streets and Alleys
Janet Attarian
Chicago Department of Transportation

Panel Discussion
Moderated by Dennis O'Brien, Jacobs Consultancy

Solar Cells and Thermoelectrics

Chair: Siddhartha Ghosh, University of Illinois at Chicago

Monday, October 5, 9:30am – 12:00pm

Solar Cells Based on CdTe Thin Film and Composite of Organic and Inorganic Nano-scale Materials
Ms. Hyeson Jung, University of Illinois at Chicago

Energy Harvesting Using Piezoelectric Materials – A Review
Dr. Banani Sen and Dr. Mitra Dutta, University of Illinois at Chicago

Analysis of the Fundamental Structure-Property Relationships in Thermoelectric $Ca_3Co_4O_9$
Professor Robert Klie, University of Illinois at Chicago

University of Illinois at Urbana-Champaign (UIUC) Research on Sustainable Energy

Chair: Charles M. Schroeder, UIUC

Monday, October 5, 1:00-5:00pm

Reconstitution of an Enzyme Mixture from the Fiber Degrading Rumen Bacterium, *Prevotella bryantii* $B_1$4 which is Capable of Deconstructing Hemicellulose

Dylan Dodd[1,2,3], Shinichi Kiyonari[2,3], Yejun Han[2,3], Charles M. Schroeder[2,3,4], Roderick I. Mackie[2,3,5], Isaac K. O. Cann[1,2,3,5]

[1]Department of Microbiology, [2]Institute for Genomic Biology, [3]Energy Biosciences Institute, [4]Department of Chemical and Biomolecular Engineering, and [5]Department of Animal Sciences, UIUC

The major target for lignocellulosic ethanol production is cellulose, a highly homogenous polymer of glucose linked together in β-1,4-glycosidic linkages. In complex with cellulose, and constituting the next highest component of plant cell wall is the more heterogeneous component, hemicellulose. Xylan is the most dominant hemicellulosic polysaccharides and xylans are composed primarily of the five-carbon sugars xylose and arabinose. Xylans have a β-1,4-linked xylose backbone that may be decorated with side chains of arabinofuranosyl, acetyl, and 4-*O*-methyl glucuronyl groups. Complete hydrolysis of xylan, thus, requires a complex set of enzymes. Microorganisms that inhabit the large first stomach of ruminants have evolved to breakdown plant fiber for subsequent fermentation to short chain fatty acids that serve as the primary energy source for the host animal. Among the rumen microbes are those specialized in the degradation of cellulose or hemicellulose, and also generalists that hydrolyze both substrates. To assemble an enzyme mixture that can deconstruct xylan, we demonstrated that the rumen bacterium *Prevotella bryantii* $B_1$4 grows rapidly on hemicellulosic substrates, such as wheat arabinoxylan (WAX). Using bioinformatics analyses of the genome sequence for this bacterium, we identified a number of genes related to hemicellulose deconstruction. Several of these genes, including an endoxylanase, an arabinofuranosidase, two β-xylosidases, an acetyl xylan esterase, and an α-glucuronidase, were expressed in large quantities as recombinant proteins in *Escherichia coli.* Experiments aimed at examining the synergistic activities of the *P. bryantii* enzymes have allowed us to reconstitute an enzyme mixture that completely degrades wheat arabinoxylan into its component sugars. The xylose fraction of this hydrolysate was efficiently converted to ethanol by the pentose metabolizing yeast, *Pichia stipitis*. This enzyme mixture represents a promising product in the current efforts to deconstruct fiber-based products for direct, efficient fermentation to biofuels.

Recombinant Yeast Strains Towards Consolidated Bioprocessing: Surface Display of Functional Mini-cellulosomes for Direct Conversion of Cellulose to Ethanol

Fei Wen, Jie Sun, and Huimin Zhao

Department of Chemical and Biomolecular Engineering, Department of Chemistry, Department of Biochemistry, Department of Bioengineering, Institute for Genomic Biology, and Center for Biophysics and Computational Biology, UIUC

Lignocellulosic biofuels represent a sustainable, renewable, and the only foreseeable alternative energy source to transportation fossil fuels. However, the recalcitrant crystalline structure of cellulosic biomass, which endows plant cell walls with resistance to biodegradation, has impeded biological production of cellulosic ethanol. The rate-limiting step in cellulosic ethanol production is the conversion of cellulose to ethanol. The current prevailing strategy to overcome this difficult step involves enzymatic hydrolysis of cellulose to glucose followed by fermentation using ethanogenic microorganisms, such as yeast *S. cerevisiae*. However, the high cost of producing large amounts of cellulases has made the cellulosic ethanol too expensive to compete with gasoline in the market. Therefore, consolidated bioprocessing (CBP), which combines enzyme production, cellulose hydrolysis, and fermentation in a single step, has been proposed to significantly lower the cellulosic ethanol production cost. Unfortunately, the great potential of CBP cannot be realized using microorganisms available today since they can not simultaneously break down cellulose to glucose and ferment it into ethanol.

In an effort to develop a CBP-enabling microorganism, we engineered a recombinant cellulolytic yeast strain by displaying mini-cellulosome on the surface. The mini-cellulosome is formed by co-expressing a mini-scaffoldin derived from *C. thermocellum* and three types of cellulases - an endoglucanase, a cellobiohydrolase, and a β-glucosidase. And the multi-enzyme complex is tethered to the yeast cell surface using the a-agglutinin adhesion receptor. The surface expression of the mini-cellulosome was confirmed and each type of cellulases in the mini-cellulosome showed respective enzymatic activity using various detection methods. Furthermore, the mini-cellulosome showed both enzyme-enzyme synergy and enzyme proximity synergy, and it was stable at 4˚C for at least four months. More importantly, yeast cells displaying the mini-cellulosome could directly convert amorphous cellulose to ethanol; and they also showed activity towards crystalline cellulose. The evaluation of ethanol production from crystalline cellulose is in progress.

Engineering an L-arabinose/xylose Co-utilizing S. cerevisiae for Biofuels Production

Tae-Hee Lee and Huimin Zhao

Department of Chemical and Biomolecular Engineering, Department of Chemistry, Department of Biochemistry, Department of Bioengineering, Institute for Genomic Biology, and Center for Biophysics and Computational Biology, UIUC

Microbial Synthesis of Xylitol from Hemicellulose

Ryan Sullivan and Huimin Zhao

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Improved utilization of hemicellulose sugars (specifically D-xylose and L-arabinose) for biosynthesis of value-added products is crucial for fermentative processes to become more economically feasible. In yeast and filamentous fungi, both pentose sugars enter the pentose phosphate pathway (PPP) through a common intermediate, xylitol, which is a five carbon sugar alcohol with a growing market as a sweetener and an important building block chemical. D-xylose is converted to xylitol through a single redox reaction by xylose reductase, while L-arabinose conversion requires a series of three redox reactions by xylose reductase, L-arabinitol 4-dehydrogenase, and L-xylulose reductase. These redox reactions require alternative forms of nicotinamide cofactor, as the reductases typically favor reduced NADPH and the dehydrogenase favors oxidized NAD^+. This results in a cofactor imbalance that potentially prohibits the efficient co-utilization of both hemicellulose sugars into xylitol.

This work describes the engineering of the first $NADP^+$-dependent L-arabinitol 4-dehydrogenase for production of xylitol from D-xylose and L-arabinose. The cofactor reversal of L-arabinitol 4-dehydrogenase by rational design and directed evolution was accomplished in an attempt to partially relieve the cofactor imbalance involved in conversion of L-arabinose to xylitol. Bioreactor studies of the xylitol pathway in *Escherichia coli* as a model organism show evidence that the engineered pathway is more efficient that the wild-type in the production of xylitol from both pentose sugars.

Electrode Characterization Using an Alkaline Microfluidic H_2/O_2 Fuel Cell as an Analytical Platform

Matt S. Naughton, Fikile R. Brushett, and Paul J. A. Kenis

Department of Chemical & Biomolecular Engineering, UIUC

Fuel cells are promising power sources due to their ability to bypass Carnot efficiency limitations by directly converting chemical energy into electrical energy. However, for significant reductions in costs and improvements in component durability must be achieved for widespread implementation of fuel cell technologies. At present, the processes that govern individual component performance and degradation *within an operating fuel cell* remain poorly understood and few analytical platforms exist to probe these complex phenomena [1]. To address this need, we have developed microfluidic fuel cells with a flowing aqueous electrolyte stream instead of a stationary polymeric membrane [2]. The constantly refreshing electrolyte stream eliminates water management issues (electrode flooding / dry-out), facilitates by-product removal and enables autonomous control of electrolyte parameters (*e.g.,* flow rate, composition). In addition, placing a reference electrode at the electrolyte outlet enables independent *in-situ* analysis of the individual electrodes, rendering this microfluidic fuel cell an excellent catalyst/electrode characterization platform.

Operating fuel cells in alkaline media, as opposed to acidic media, is advantageous as enhanced fuel oxidation and oxygen reduction kinetics improve fuel cell energetic efficiency [3]. Furthermore, cheap non-precious metal catalysts, *i.e.* silver (Ag) cathodes and nickel (Ni) anodes, may be used in place of expensive Pt-based catalysts without significant performance reduction. Unfortunately, carbonate formation, occurring when hydroxyl ions react with carbon dioxide from organic fuel oxidation and/or from the ambient environment, remains a significant technical challenge [4-6]. Traditional alkaline fuel cells (AFCs) utilize a stationary alkaline electrolyte which is relatively inexpensive but more vulnerable to carbonate precipitation which reduces electrolyte conductivity and deactivate electrodes. Alkaline anion exchange membrane (AAEM)-based fuel cells are less susceptible to carbonate precipitation due to the lack of a mobile cation [7], but are hindered by membrane costs and performance limitations notably water management and unfavorable pH gradients [8]. Furthermore, the inherent alkalinity of an AAEM limits ways to fine tune electrolyte composition with respect to optimizing electrode reaction kinetics (*e.g.*, optimize pH).

Here, we present research on the effects of electrolyte composition (*e.g.,* pH, [carbonate]) on the Pt/C and Ag/C electrode performance in an alkaline microfluidic H_2/O_2 fuel cell. Precise control over electrolyte parameters enables *in-situ* analysis of electrode and fuel cell performance without disassembly. Optimal hydrogen oxidation and oxygen reduction reaction conditions are investigated by varying alkaline electrolyte concentrations. Carbonate formation effects are studied by altering hydroxide and carbonate ion ratios in the electrolyte stream. Understanding AFC electrode performances will enable membrane-electrode assembly (MEA) optimization and provide valuable insight for developing alkaline direct liquid fuel cells.

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Perspectives on Energy and Sustainability

Chair: George Crabtree, Materials Science Division, Argonne National Laboratory

Monday, October 5, 1:00-5:00pm

The Energy and Sustainability Challenges

George Crabtree
Materials Science Division, Argonne National Laboratory

The global dependence on fossil fuels is among the greatest challenges facing our economic, social and political future. The uncertainty in the cost and supply of oil threatens the global economy and our national energy security, and the emission of pollutants and greenhouse gases threatens the environment and global climate. The transition to greater sustainability involves tapping unused energy flows such as sunlight and wind, producing electricity without carbon emissions from clean coal and high efficiency nuclear power plants, and using energy more efficiently. Achieving these goals requires creating new materials with greater complexity and functionality to control the transformation of energy among light, electrons and chemical bonds. The sustainability of next generation energy technologies will be evaluated, the roadblocks to their implementation will be described, and the scientific and technical breakthroughs needed to overcome the roadblocks will be presented.

Chicago's Vision for Energy and Sustainability

David O'Donnell, Deputy Commissioner
Dana Kenney, Assistant Commissioner
Department of the Environment, City of Chicago

The Chicago Climate Action Plan, a comprehensive plan for both mitigating and adapting to climate change, will be presented. The plan recognizes the key role that both energy efficiency and renewable energy play in a sustainable energy future for the City's residents and businesses. The presentation will discuss both the carbon footprint of Chicago energy uses as well as initiatives underway to improve the sustainability of Chicago's energy future.

More information on the Chicago Climate Action Plan can be found at http://www.chicagoclimateaction.org/pages/chicago_climate_action_plan/45.php

The Initiative for Sustainability and Energy at Northwestern University

David C. Dunand
Department of Materials Science and Engineering, Northwestern University

Worldwide, universities are becoming deeply involved in the issue of energy and sustainability, contributing in terms of research, teaching and outreach. At Northwestern University, President Henry Bienen launched in October 2008 the Initiative Sustainability and Energy at Northwestern (ISEN). The mission of ISEN is to create, advance and communicate new science, technology, and policy for sustainability and energy, with a particular focus on sustainable energy supply, demand and use. Within Northwestern University, ISEN serves as: (i) a catalyst for new research in this field, (ii) a unifying force for targeted teaching in this area, and (iii) a hub for outreach activities. Examples for all three of these missions are given, and plans for future activities are presented.

Sustainability in the Urban University

Cynthia (Cindy) Klein-Banai
Associate Chancellor for Sustainability, University of Illinois at Chicago

There are a growing number of examples of how universities are becoming more sustainable, particularly in their use of energy. Although there has been an historic recognition that universities should be "greener", this has mostly been manifested through programs such as recycling and lighting retrofits. In 2001, the Association for Advancement of Sustainability in Higher Education and the American College & University Presidents' Climate Commitment are two national organizations which provide resources to member institutions with a goal of making campuses more sustainable, to neutralize greenhouse gas emissions, and to enhance the research and educational efforts of higher education to equip society to address climate change. There are already examples of universities and colleges such as Middlebury College, the University of Minnesota, Morris and the University of New Hampshire that have made huge strides to becoming climate neutral – through biomass, wind energy and landfill gas. These are rural campuses, however, not urban universities like UIC. UIC is both constrained and benefited by being part of the third largest city in the U.S. There is access to all types of public transit, biking, and walking, but an urban location is not appropriate for siting large wind turbines that can produce renewable energy. Our land footprint is small compared to our population, but we don't have acres of forests to off-set our carbon emissions. We have access to all kinds of recycling contractors and can take advantage of Chicago's C&D ordinance, but we don't have space for a large compost operation. Chicago is in a non-attainment zone for ozone and particulates, limiting the potential fuels for our power plants. However, UIC also burns a cleaner fuel than coal campus because of permit constraints. How does an urban university, like UIC, plan to become climate neutral? It leverages its current activities with those of the city and innovates.

The Business of Sustainability:
The balance between profit and progress…

Peter Dreiske
Senior Director of Photovoltaic Devices and Systems
EPIR Technologies, Inc

Due to ever increasing demands for energy to power our homes, transportation, agriculture, and businesses, the cost and availability of energy is becoming of critical importance in the health of our economies; whether local, national, or global. A fundamental component of these economies are the businesses, from small to large, that provide goods, services, and technology; and of course, employment. Therefore, the health of businesses and our economy can no longer be separated from the cost of energy. At the core of these mutually interconnected components is the actual business of providing this energy. In this nucleus is where the collision between profitability and progress occurs; the profound question of economics versus environment, and the ideological boundary between left and right. Further, the business of energy is now at the very forefront of competition between nations; for countries to become and/or remain healthy they must address the near and long term endurance of their energy technology and policy in an increasingly competitive environment. The long term endurance of an energy technology (or business) to provide power at low cost, sufficient quantity, and reduced "side effects" is at the very heart of sustainability. This talk will attempt to present the interrelationships between the various components discussed in this abstract, the opportunities and challenges faced, and if not provide complete answers, at least frame the questions for the "Business of Sustainability"…

Future Electrical Energy Generation and Distribution

Chair: Kevin Taylor, Detroit AIChE, IEEE

Monday, October 5, 1:00-5:00 pm

Session Description

Sustainable is the environmentally friendly buzzword of the current decade. In the past, electrical power generation is not something commonly associated with "being green." The session covers some of the latest technical developments in control and production of renewable power. The papers presented cover not only the more common renewable power generation options; but the practical implementation of alternate energy technologies that create challenges to the planners of our distribution and transmission electric system.

The Potential of Smart Grid in Illinois

Jim Crane
ComEd

This presentation will discuss the impact of federal and state smart grid initiatives to drive change in the electric utility industry in Illinois. Federal funding from the American Recovery and Reinvestment Act of 2009 (ARRA) along with the Energy Independence and Security Act (EISA) of 2007 could have a dramatic impact on Illinoisans Some $4.3 billion in federal funding is available for smart grid applications and is poised to transform the electric utility industry. New customer applications and choice will transform the way Americans use energy and interact with their electric utility providers. Modernization of the transmission and distribution system will improve reliability and enable new customer applications and choice. New policies and rate recovery mechanisms will be needed to support these applications and Illinois is positioned to be at the forefront of the smart grid revolution.

Wind Forecasting and Integration into Power System Operations

Jianhui Wang Ph.D
Decision and Information Sciences Division
Argonne National Laboratory

This talk is to discuss wind power forecasting and its use in power system operations. The presentation is structured into two parts. The first part concentrates on surveying existing wind power forecasting methodologies and identifying strengths and limitations of different approaches. The second part of the presentation addresses how power system operators can incorporate advanced wind forecasting technologies into their operations. Improved unit commitment and dispatch algorithms to address variability and uncertainty of wind power will be discussed.

Minimization of Water Consumption Under Uncertainty for Pulverized Coal (PC) Process

Juan M. Salazar, Research Engineer
Urmila M. Diwekar, President,
Vishwamitra Research Institute: Center for Uncertain Systems Tools for Optimization and Management
Collaboratory for Process & Dynamic Systems Research, National Energy Technology Laboratory

Coal-fired power plants are large water consumers second only to agricultural irrigation. Water restrictions become more influential when water-expensive carbon sequestration 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 thermoelectric generation is strongly associated to evaporation losses and makeup streams on cooling and contaminant removal systems. Thus, minimization of water consumption requires optimal operating conditions and parameters, while fulfilling the environmental constraints.

Several uncertainties affect the operation of the plants and this work studies those associated to weather. Air conditions (temperature and humidity) were included as uncertain factors for pulverized coal (PC) power plants. The study comprises three main steps: Characterization of uncertainty, sensitivity analysis and optimization. Probability distributions were obtained from available atmospheric and electric generation data. The distributions characterize air conditions and electricity demand variability as uncertain factors. A stochastic simulation capability in the Aspen Plus process simulator was employed to perform sensitivity analysis and to determine the decision variables for the final step. Optimization under uncertainty for these large-scale complex processes with black-box models cannot be solved with conventional stochastic programming algorithms because of the large computational expense. Employment of the novel better optimization of nonlinear uncertain systems (BONUS) algorithm, also implemented as an Aspen Plus capability, dramatically decreased the computational requirements of the stochastic optimization. Operating conditions including reactor temperatures and pressures; reactant ratios and conditions; and steam flowrates and conditions were calculated to obtain the minimum water consumption under the above mentioned uncertainties. Reductions of up to 12% in water consumption were calculated when process variables were set to optimal values.

Stochastic Modeling of Biodiesel Production Process

Sheraz Abbasi and Urmila Diwekar
University of Illinois -Chicago

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.

Biomass Energy

Chair: Terry Marker, Gas Technology Institute

Tuesday, October 6, 9:30am - 12:00pm

Biomass Gasification

Michael Roberts
Gas Technology Institute

Biomass is a renewable resource that can be gasified to produce synthesis gases suitable for the production of clean power, chemicals, and/or fuels. Efforts in the U.S. and around the world to reduce production of greenhouse gases and carbon footprints are impacting the way power is generated. In addition renewable portfolio considerations in the U.S., Britain, Italy, and Belgium have provided a significant boost to interest in renewable energy from wind, hydro, biomass and other technologies.

Biomass gasification can be accomplished in fixed bed, fluid bed and/or entrained bed gasifiers with each type of gasifier possessing certain advantages and disadvantages inherent to its design. All biomass gasifiers generate tars to some degree; tar removal and general gas cleanup must be incorporated in overall designs to provide clean synthesis gas to downstream processes. Ultimately, widespread adoption of a green energy agenda and bio-derived fuels are driven by tax incentives and portfolio standards.

Glass-Ceramic Catalysts for Tar Decomposition in Biomass Gasification

Logan Weast,
Gas Technology Institute

The harsh environment and high temperatures in a fluidized bed biomass gasifier require the use of robust bed materials, and cleanup of the product gas typically requires additional downstream processing. In an effort to streamline this process and reduce the costs associated with gas cleanup, the Gas Technology Institute has developed several novel glass-ceramic catalyst materials capable of actively decomposing tar compounds while in the fluidized bed reactor.

Glass-ceramics are materials which are initially formulated and formed as glass articles and then subsequently treated in a controlled heating process to form typically fine-grained ceramic articles. By careful selection of the formulation and heat treatment parameters, catalyst materials have been created that possess high melting points (>1200 ℃), exceptional attrition resistance, and strong catalytic activity for tar decomposition. This presentation will discuss the process in which lithium- and magnesium-aluminosilicate glasses containing up to 40 wt% transition metal oxides have been treated to form multi-phase fine-grained ceramics. These ceramics have then been subjected to reducing conditions, which reveals an active metal layer at their surface. Also, we compare the decomposition activity and physical properties of these novel catalysts with

minerals such as olivine and dolomite which are more commonly used as high temperature fluidized bed media.

Integrated Hydropyrolysis and Hydroconversion Process for Production of Gasoline and Diesel Fuel from Biomass

Terry Marker, Larry Felix and *Martin Linck*
Gas Technology Institute

Experimental results and a process design will be presented for an integrated process which uses hydropyrolysis plus hydroconversion to convert biomass into gasoline and diesel. The hydrogen needed for the hydropyrolysis and hydroconversion process is produced by reforming the light gases so that no external H2 is required. Finished hydrocarbon products with less than 2% oxygen are produced using this processing approach. This approach is superior to conventional pyrolysis, in that a chemically stable, deoxygenated hydrocarbon product is obtained.

Biogas Cleanup and Use

Ted Barnes, P.E.
Advanced Energy Systems
Gas Technology Institute

Businesses and municipalities across the country are trying to come to terms with increasing, unstable energy prices and escalating costs for waste removal. There is an immediate need for solutions that provide renewable, inexpensive, and domestically produced energy sources that can be implemented in the near-term. Biogas can be generated from various feedstocks (agricultural waste, waste water, landfills, etc.) and used to supply numerous energy needs including electricity and vehicle fuels. With the right clean-up and conversion technologies, biogas systems can be flexible enough to be applied in many different industries and provide solutions based on a specific location's waste streams and energy needs.

In order to produce a useful, energy-rich product, it is typically necessary to separate the high-energy methane from the undesirable compounds in a biogas composition. Since no two sites yield biogas with exactly the same composition, the system design must be based on a detailed analysis of a given location. GTI has been involved in the design of a variety of biogas cleanup systems. One such project entails the conversion of agricultural waste to biogas at Gills Onions, an onion processing plant in Oxnard, CA that generates approximately 300,000 lbs of waste per day. The biogas is used to generate ultra-clean electricity in two 300 kW molten carbonate fuel cells. Before the biogas can be sent to the fuel cell's reformer it must be purified to reduce its concentration of sulfur compounds from approximately 5000 ppm to less than 1 ppm. Another GTI cleanup project involves biogas from a waste water treatment plant at the U.S. Army's Forces Command, in Fort Lewis, WA. The purified gas will be used to produce hydrogen for fueling 19 fuel cell powered forklifts and a fuel cell hybrid electric bus on the base. The final project that will be discussed is the cleanup and liquefaction of landfill gas at the Altamont landfill in Livermore, CA. The landfill gas is put through a conditioning and cleanup system before it is cooled to cryogenic levels to produce 13,000 gallons per day of liquefied natural gas (LNG) that will be used to run waste haulers throughout California.

Catalysis for Energy

Chair: Randall Meyer, University of Illinois at Chicago

Tuesday, October 6, 9:30am – 12:00pm

Energy Efficient Catalysts and Processes for the Petrochemical Industry: Future Challenges in Energy

Javier Guzman, Mike Bedell, and Bruce R. Cook,
Advanced Refining, BP North America

Global energy demand and environmental concerns will continue to grow in the next decades, motivating the petrochemical industry to search for new more efficient chemical process technologies; in particular for the production of transportation fuels and value-added chemicals which are ecologically sustainable and economically viable. Many technology platforms, including solar, wind, nuclear, biomass- and hydrogen-based, have been proposed as alternatives to the use of fossil fuels. Although these technologies are promising and resources are being directed toward their industrial development, their volume contribution to the total energy supply will represent no more than 25% by 2030. Oil, gas, and coal will continue to support a high percentage of the world's energy demand in the future. This talk will present an industrial perspective of energy, chemical processes, advanced catalysts, and their interrelationships; addressing the catalysis challenges for the next decades.

Kinetic Monte Carlo Simulation for ($\sqrt{5}$x$\sqrt{5}$)R27° Surface Oxide over Pd(100)

Jelena Jelic[1], Randall Meyer[1], Karsten Reuter[2]
[1]*Department of Chemical Engineering, University of Illinois at Chicago,*
[2] *Fritz Haber Institute*

Under realistic operating conditions, in heterogeneous oxidation catalysts, the active surface for catalysis may actually be a surface oxide instead of a pristine, metal surface. We used Density Functional theory to investigate the stability of Pd(100) and Pd(111) surfaces under NO oxidation conditions, for various oxygen and NO pressures at 600K. Under conditions of interest (P_{O2} =1 bar and P_{NO} =1mbar) according to thermodynamic phase diagram, Pd should be oxidized completely to be bulk palladium oxide. However, kinetic limitations may exist such that its formation is slow compared to the cycling of NOx Storage Reduction systems. To further investigate this point, first principles kinetic Monte Carlo (kMC) simulations were performed which combine an accurate description of the elementary processes (using DFT theory to obtain the kinetic parameters of the individual processes) and account for their statistical interplay over an extended time scale in order to properly evaluate the surface chemical kinetics. KMC simulations are performed in order to check the stability of the PdO(101) surface oxide over Pd(100) under relevant NO oxidation conditions and to determine TOF values over a wide range of temperature and pressure conditions. From these results we conclude that the surface oxide of PdO(101) is a reasonable model for Pd NO oxidation catalysts under the lean cycle of NOx storage reduction. Our results further suggest that other metals which oxidize easily may still be viable candidates for NOx storage systems and may improve the low temperature NO oxidation activity.

In-situ XAFS analysis for the synthesis and testing of supported Pt catalysts for propane oxidation

Worajit Setthapun[1], Jeffrey W. Elam[2], Federico A. Rabuffetti[3], James A. Enterkin[3], Kenneth R. Poeppelmeier[3], Laurence D. Marks[4], Peter C. Stair[1,3], Jeffrey T. Miller[1], and Christopher L. Marshall[1]

[1]*Chemical Sciences and Engineering Division, Argonne National Laboratory*
[2]*Energy System Division, Argonne National Laboratory*
[3]*Department of Chemistry, Northwestern University*
[4]*Department of Materials Science and Engineering, Northwestern University*

Highly uniform Pt nanoparticles coated over γ-Al_2O_3, spherical-Al_2O_3 and $SrTiO_3$ nanocube catalysts were synthesized by using Atomic Layer Deposition method (ALD). The Pt particles were extremely uniform in size and fully disperse on the surface of oxide supports. Using ALD to deposit Pt over oxide support is not a conventional method in heterogeneous catalyst synthesis. ALD technique was mainly used in the semiconductor industries to synthesize thin films. In this work, the mechanism of Pt ALD was studied in each ALD step. In-situ X-ray absorption fine-structure (XAFS) was used to determine the mechanism of the Pt nanoparticle formation over the oxide supports mainly γ-Al_2O_3.

Platinum-based catalysts are known to be highly active for the deep oxidation of hydrocarbons. However, typical catalysts such as Pt/□-Al_2O_3 require relatively high temperatures in order to completely oxidize lower alkanes such as ethane or propane. Pt/$SrTiO_3$ has significantly higher propane turn over frequency (TOF) than the standard Pt/□-Al_2O_3 catalyst. Pt/$SrTiO_3$ is a very robust catalyst and does not need pretreatment prior to catalytic testing. It can also withstand several temperature cycles without exhibiting activity change. The correlation between Pt loading, Pt oxidation state, light-off temperature and propane TOF will be presented. The oxidation state of the Pt nanoparticles during propane oxidation were determine by in-situ XAFS.

Selective Adsorption of Manganese onto Cobalt for Optimized Mn/Co/TiO_2 Fischer-Tropsch Catalysts

Theresa Feltes[1], Randall Meyer[1], Bert Weckhuysen[2], John Regalbuto[1]
[1]*Department of Chemical Engineering, University of Illinois at Chicago*
[2]*Inorganic Chemistry and Catalysis, Utrecht University*

Manganese promoted Cobalt Fischer-Tropsch (FT) catalysts have been shown to have higher CO conversion and enhanced selectivity towards C_{5+} hydrocarbon chains especially when the MnO particles are in close interaction with the Co^0, inducing an electronic promotion effect [1]. Until now, controlled intimate contact between the Co^0 and MnO particles has proven difficult to achieve, since current synthesis methods often lead to inconsistent and random distribution of the promoter over the catalyst surface.

By controlling the charging parameters of the hydroxyl groups on an oxide support via pH, Regalbuto et al. have shown that a metal complex can be strongly adsorbed on to the oxide surface with high dispersion [2]. Schwarz proposed years ago that one could utilize these electrostatic interactions to direct the adsorption of a metal onto the precursor oxide phase of a supported metal catalyst rather than the support to achieve selective adsorption [3]. Application of this technique can be very beneficial in promoted metal catalysts where intimate contact between the active metal and promoter oxide is of fundamental importance.

This work applies the theory of selective adsorption to the synthesis of Mn/Co/TiO_2 FT catalysts by driving the manganese on to the supported Co_3O_4 phase to achieve systematic catalyst preparation for reaction. Characterization and FT reactivity measurements of these catalysts have presented a more qualitative and quantitative understanding of the effect manganese has on the supported cobalt catalyst.

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[3] Schwarz, J.A., Ugbor, C.T., and Zhang, R., *J Catal.* 138, 38 (1992).

Glycosidic Bond Cleavage in Oxidative Hydrolysis of Cellulosic Materials

Weiling Deng[1], Sungsik Lee[1], Stefan Vajda[1], Joseph A. Libera[2], Jeffrey W. Elam[2], and Christopher L. Marshall[1]

[1]Chemical Sciences and Engineering Division, Argonne National Laboratory
[2]Energy Systems Division, Argonne National Laboratory

Renewable biofuel and chemical production from the degradation of biomass (such as cellulose) is one of the grand challenges. New research has focused on C-O-C bond cleavage in cellulosic materials in an oxidizing condition by heterogeneous catalysis, as contrast to conventional breakdown of cellulose including expensive enzymatic process or concentrated sulfuric acid treatment. Model compounds with appropriate C-O-C linkages are used to understand the reaction pathways and changes in catalyst morphology that lead to the oxidative breakdown of cellulose. Nanometer and sub-nanometer metal catalysts (Pd, Pt, VOx, Co) were found to be able to break the C-O-C bond, producing alcohols, or to form ketones by further oxidation. The effect of contact time on catalyst activity and tuning selectivity was confirmed by changing the metal cluster location from the flow channel entrance to the exit. Research results from more realistic feed conditions of cellulose demonstrate that air-assisted hydrolysis of cellobiose is able to obtain over 70% glucose yield. This sheds new light on a more environmentally friendly way to converting cellulose to monosaccharide sugars.

Catalysis for the Generation of Biofuels

William C Ketchie and Joseph A. Kocal
UOP LLC – A Honeywell Company

There are many driving forces for the continued development and utilization of second generation biofuels. Two keys to the development of such biofuels are emphasis on the life cycle of the feedstock as a measure of sustainability and generating technologies that are feedstock flexible. The sustainability of a few potential bridging and second generation biofuel feed sources, such as jatropha and algae oils, will be reviewed. These potential feedstocks have successfully been transformed into green diesel and jet fuel using UOP/ENI's Ecofining™ process and UOP's Renewable Jet Fuel process. The Ecofining™ process utilizes heterogeneous catalysts to convert natural oils via deoxygenation and isomerization reactions into a high quality green diesel or jet product. Green diesel offers many advantages over traditional biodiesel (fatty acid methyl ester), such as zero oxygen content, better cold flow properties and oxidative stability. The UOP Renewable Jet process yields a fuel that meets all of the ASTM standards for aviation fuels. The UOP Renewable Jet Fuel process incorporates a selective cracking reaction step to enable the generation of green jet fuel from the natural oils and greases to meet the stringent specifications.

Medical Imaging Advances

Chair: Don Chmielewski, IIT

Tuesday, October 6, 9:30am – 12:00pm

Development of a Magnetic Resonance Diffusion Tensor template of the Human Brain

Konstantinos Arfanakis, BME Department, IIT

Diffusion tensor imaging (DTI), by means of magnetic resonance imaging (MRI), is unique in providing a wealth of information regarding the microstructure of brain tissue in vivo. Voxel-based comparisons of neuronal structural integrity and brain connectivity across populations require accurate spatial normalization of DTI data between subjects. This, in turn, requires an accurate brain template. In this presentation, the effects of DTI data acquisition, image reconstruction, image registration, and different summary statistics, on the accuracy of the final brain template, will be discussed.

Automated Image Diagnostic-Quality Characterization

Jovan Brankov, ECE Department, IIT

There is a critical need in the imaging field for a reliable approach to judge the quality of images produced by an imaging device or algorithm. This is necessary for optimization and testing of imaging technologies of all kinds. A strong consensus is emerging in the medical-imaging community that image quality should be defined in terms of the performance of an observer on some clinically relevant task (i.e., an image is “good” if it causes physicians to produce accurate diagnoses of their patients). Thus, the gold standard is the human-observer study, an experiment in which physicians’ performance is measured statistically. However, this approach is impractical in most situations. Therefore, numerical observers—algorithms that emulate human observer performance — are badly needed as a guide to developing new imaging technologies.

In this talk, a suite of numerical observers will be described that uses state-of-the-art techniques from pattern recognition and machine learning to predict human-observer performance based on images. Our approach has already been adopted by industry, and we started an NIH-sponsored project to develop this approach for the benefit of the greater imaging field. Our approach represents a major paradigm shift in this field, and we will show in the talk that it outperforms traditional approaches for making image-quality assessments.

Phase-Contrast Imaging and the Potential for Low-Dose Mammography

Adam Zysk, ECE Department, IIT

Phase-contrast imaging derives contrast from the refractive index of an object instead of the absorption, as is common in traditional radiography. This mechanism has recently been applied to a number of radiographic tasks for visualization of soft tissue structures that are typically invisible in traditional x-ray images. Since phase-contrast persists at high x-ray energies where the absorbed dose is low, there may also be potential to apply phase-contrast techniques to mammography in order to reduce dose. The development of an experimental phase-contrast x-ray system, the simulation of clinical images, and the evaluation of low-dose contrast will be discussed.

Limited Data Image Reconstruction in Photoacoustic Tomography

Kun Wang, BME Department, IIT

Photoacoustic tomography, is an emerging hybrid imaging technique with great potential for a wide range of biomedical imaging applications. Mathematically exact algorithms are available for image reconstruction, but they are applicable only when the measured data are densely sampled on an aperture that encloses the object. In many cases of practical interest, however, measurements may be limited in number and are acquired on an incomplete aperture. In this work, we develop and investigate an iterative reconstruction algorithm for limited-data TAT. The algorithm is based on the minimization of the image total variation (TV), and is conceptually and mathematically distinct from classic iterative reconstruction algorithms. Computer-simulation studies are conducted to investigate the proposed algorithm. These studies reveal that the TV-based algorithmcan yield accurate reconstructions in many limited-data applications where classic iterative algorithms do not perform well.

Alternative Fuels

Chair: Pat Shannon, Middough

Session Description

Biologically-derived fuels are assuming increasing importance in the U.S. Administration's attempts to reduce dependence on imported oil. While this is encouraging, some problems do exist. For example, the basic chemistry and biology mechanisms for viable alternative fuels production are not well understood. There has already been marked pressure on food prices as more agricultural products are diverted to fuels production. And the long-term economic and environmental sustainability of several of the established processes is unclear.

Tuesday, October 6, 1:00 – 5:00pm

Inhibition of the Switch from Glucose to Xylose by Ethanol Concentration: The Advantage of the Cell Recycle

P.J. Slininger
National Center for Agricultural Utilization Research, USDA-ARS

To expand the biomass to fuel ethanol industry, process strategies are needed to breakdown lignocellulose to fermentable sugars and to foster the production of microorganisms which can survive and ferment the resulting hexose and pentose sugars while exposed to inhibitors such as ethanol. In hydrolyzates, the switch from glucose to xylose uptake can result in diauxic lag unless steps are taken to prevent this. The use of recycled cells can eliminate diauxy if cells are appropriately conditioned. When cells were primed on glucose, the length of this lag was a function of the glucose concentration consumed (and the ethanol concentration accumulated) prior to the switch from glucose to xylose fermentation. The impact of ethanol on enzyme induction and the length of diauxy was explored. Priming recycled cells with a high xylose concentration was observed to induce faster fermentation rates and to eliminate diauxic lag during mixed sugar conversion by *P. stipitis* NRRL Y-7124 despite ethanol accumulations exceeding 60 g/L. Process strategies to lower the cost of ethanol from biomass are suggested by the results of this work.

Biomass fuel for Combined Heat and Power

Dean Karafa
Middough

The University of Illinois is currently designing a Combined Heat and Power (CHP) demonstration plant that will use a highly touted energy crop, Miscanthus x giganteus (Miscanthus) as the fuel source. It is hoped that Miscanthus can become an integral component of a sustainable energy

supply chain. To better understand the integration of Miscanthus with an energy system, the University will be installing a boiler that will generate steam from the combustion of Miscanthus and then use that steam to generate power in a steam turbine generator.
This presentation will discuss the characteristics of the energy crop with respect to combustion, the equipment and systems to be installed at the University, and the expected performance of the fully integrated system.

GLBRC Thrust 2 Efforts to Deconstruction Plant Cell Wall to Fermentable Sugars and Fuel Molecules

Venkatesh Balan and Bruce Dale
Great Lakes Bioenergy Center, Michigan State University

Developing robust, affordable, and sustainable fuels is the single greatest technical challenge facing our country and the world. Without these developments over the next several dozen years, the United States risks continued dependence on foreign and non-renewable energy and all of the accompanying risks to the country's economic and political security. The world risks the serious ecological consequences of global warming and economic upheaval. The GLBRC is the only university-based Bioenergy Research Center funded by DOE. It has the highly applied mission to enable sustainable biofuels production through fundamental research, and is dependent on the creative basic science environment inherent to major research universities. It has responsibilities in both research and education, and must operate using a hybrid strategy that combines the inherent strengths of academic science with the timelines and milestones required for applied science. The four research thrusts of the Center support development of a robust pipeline from biomass production through biomass pretreatment and final conversion to fuel. The talk will primarily focus on thrust 2 which has two primary overall objectives: 1) to significantly improve the fundamental science of plant cell wall deconstruction and 2) to remove the technological roadblocks to efficient conversion at high yield, concentration and rate of plant structural carbohydrates and other plant compounds to fuel molecules and intermediates for fuel production.

Enzymes Screening and Optimization for Hydrolysis On Ammonia Fiber Expansion Treated Corn Stover

Dahai Gao, Shishir P. S. Chundawat, Bruce E. Dale and Venkatesh Balan,
Great Lakes Bioenergy Center, Michigan State University

With the depletion of non-renewable petroleum reserves, producing biofuels and biochemicals from biomass has been given significant attention to help transform the existing petroleum based economy to bio-based one. Lignocellulosic biomass provides an abundant resource for the sustainable production of fuels and chemicals. However, the high cost of hydrolytic enzymes is one of the major factors impeding the implementation of an economically viable lignocellulosic biorefinery. In order to depolymerize biomass effectively, one must have the right batter of enzymes with optimized combination.

In this study, we evaluate enzymes from bacterial and fungal sources. CBH I, CBH II and EG I are purified from commercial enzyme Spezyme CP, ßG is purified from Novozyme 188. Two cellulases (LC1 and LC2), two xylanase (LX1 and LX2), one ß-glucosidases (LßG) and one ß-xylosidases (LßX) are from bacterial sources provided by Lucigen. By swapping and doping bacterial enzymes to fungal enzymes mixture, bacterial hemicellulases show they work synergistically with fungal cellulases by increasing both glucose and xylose yields. Further studies were carried out using 73 different mixtures of the fungal and bacterial enzymes (CBH I, CBH II, EG I, bG, LX1, LX2, LbX), based on a statistical design of mixtures, to determine optimal ratios of enzymes that maximized glucose and xylose yields. The mixtures loaded at 3 different total protein loadings (10, 15 and 30 mg/g glucan) helped reconfirm the synergistic interactions between the bacterial hemicellulases and fungal cellulases. These results depict the route of screening suitable enzymes for hydrolysis and make best use of selected enzymes by optimization relative ratio which could help decrease total enzyme usage and reduce bio-fuel production costs.

Ultra-structural and Physicochemical Modifications within Ammonia Pretreated Lignocellulosic Cell Walls that Influence Enzyme Accessibility

Leonardo da Costa Sousa[1], Shishir P. S. Chundawat[1], Bryon S. Donohoe[2], Lekh Sharma[3], Thomas Elder[4], Per Askeland[1], Ramin Vismeh[5], Umesh Agarwal[6], James Humpula[1], Rebecca Garlock[1], Daniel A. Jones[5], Kevin Chambliss[3], Michael E. Himmel[2], Balan Venkatesh[1], Bruce E. Dale[1].

[1]Biomass Conversion Research Lab (BCRL), Department of Chemical Engineering & Materials Science, Michigan State University
[2]Chemical and Biosciences Center, National Renewable Energy Laboratory
[3]Department of Chemistry & Biochemistry, Baylor University
[4]USDA-Forest Service, Southern Research Station
[5]Department of Biochemistry and Molecular Biology, Michigan State University
[6]USDA-Forest Products Laboratory

We have identified the major ultra-structural and chemical modifications incorporated within plant cell walls during AFEX using several microscopic, spectroscopic and spectrometric techniques. High resolution microscopic (SEM, TEM) and 3D-EM-Tomographic studies indicate an ultra-structural alteration of AFEX treated cell walls via formation of a nanoporous tunnel-like network. Closer analysis (ESCA, AFM and confocal fluorescence microscopy) of outer cell wall surfaces shows heterogeneous deposits rich in AFEX degradation products and various other cell wall extractives (e.g. lignin, arabinoxylan rich oligomers, calcium). Raman spectral data indicates conversion of cellulose I to III is intricately dependent on AFEX pretreatment conditions (i.e. ammonia/moisture loading, residence time). More than 45 AFEX degradation products have been identified and quantified using LC-MS/MS and GC-MS methodologies. Some of the major degradation products include organic acids (lactic, acetic), aromatics (vanillin, hydroxybenzaldehyde), phenolic acids (ferulic, coumaric) and amides (acetamide, feruloyl and coumaroyl amide). This fundamental understanding of physicochemical modifications of the plant cell wall during pretreatment and its effect on enzymatic hydrolysis are critical to achieve the goal to reduce pretreatment severity and further improve the process economics. This understanding will be also important for plant biologists, which can re-engineer plant cell walls to facilitate the pretreatment action at even lower severities.

Novel Materials and Processing for Energy & Sustainability

Chair: Justin Notestein, Northwestern University

Tuesday, October 6, 1:00 – 5:00pm

Next Generation of Rechargeable Li-ion Batteries: Challenges, Opportunities, and Advances at Northwestern

Jung-Kyoo Lee, Kurt Smith, Cary Hayner, and Harold Kung*

Department of Chemical and Biological Engineering, Northwestern University

Rechargeable batteries, while widely used in small electronic devices and hand-held tools, are potentially well suited for use in battery-powered electric vehicles and for storage in power generation facilities. The hurdles for these applications include energy and power densities, durability, and cost, some of which can be overcome by using light weight materials that have high Li storage capacities for the electrodes and strong but inert ones for other battery components. A discussion of these challenges and examples of progress to resolve them, such as using nano-composites for energy storage will be presented.

Development of Nanostructured Thermoelectric Materials for More Efficient Heat-to-Power Generation

Steven N. Girard and Mercouri G. Kanatzidis

Department of Chemistry, Northwestern University

Renewable energy initiatives have increased interest in thermoelectric materials as an option for inexpensive and environmentally friendly heat-to-power generation. The efficiency of a thermoelectric material is related to its figure of merit *ZT*, defined as $ZT = S^2\sigma T/\kappa_{tot}$, where *S* is the thermopower or Seebeck coefficient, σ is the electrical conductivity, *T* is the operating temperature, and κ_{tot} is the total thermal conductivity (a sum of the electronic κ_{elec} and lattice κ_{lat} vibrations). In practice, any heat-generating process (such as the combustion of fossil fuels in cars and power plants) can be made more efficient by recouping lost waste heat. However, conventional bulk thermoelectric materials (such as PbTe, Bi_2Te_3, and SiGe) have limited utility due to maximum *ZT* values of ~0.8, corresponding to efficiencies around 5% given a temperature gradient of 350 K. By incorporating appropriate nanostructures within existing thermoelectric bulk materials, *ZT* can be enhanced due to an increase in phonon scattering that effectively reduces the lattice thermal conductivity, κ_{lat}. Corresponding *ZT* values in excess of 1.2 increase the potential utility of nanostructured bulk materials, and we demonstrate reproducibility and scalability of investigated material systems.

Titania Thin Films Prepared by Reactive Sputtering: Non-Stoichiometry and Cation Doping

Paul Desario, Le Chen, Michael Graham, Kimberly Gray

Department of Civil and Environmental Engineering, Northwestern University

A deeper understanding of the relationships between synthesis, structure and function has proved to be critical in order to improve the design of materials tailored to solar energy conversion and storage. The objective of this research is to synthesize TiO_2 nano-structured thin films with properties tailored for the photoreduction of CO_2 to CH_4 under UV and visible light. Our efforts are guided by the objectives of (a) creating a high number of photoactive sites, (b) optimizing charge separation, and (c) increasing the response to visible light for improved photo-efficiency in photocatalytic performance.

Unbalanced reactive dc magnetron sputtering (UBMS) with partial pressure control of oxygen is utilized to fabricate mixed-phase TiO_2 films with novel nanostructures, high solid-solid interfacial areas and enhanced oxidative and reductive activities. Recent studies have focused on, the role of non-stoichiometry (oxygen vacancies) and cation doping (Nb) in mixed phase titania to influence the photoresponse and photocatalytic performance. Films were deposited at different partial pressures of oxygen to yield different levels of non-stoichiometry. The non-stiochiometric films show a strong red-shift and there is an optimal non-stiochiometry for films with respect to methane yield from CO_2 reduction under UV and visible illumination. Nb-doped films ($Ti_{1-x}Nb_xO_2$) in the range of $0<x<0.45$ were also prepared to evaluate the effect of cation doping on optical, chemical and physical properties. We have determined how the addition of Nb cations changes the film growth and phase formation relative to the pure material. The shift in optical absorption to the visible wavelength range as a function of Nb concentration and anatase-rutile phase distribution is also presented, and the results suggest that the addition of Nb cations is even more effective than oxygen vacancy control alone in causing a red shift in the absorption response of the films. Our studies continue to evaluate the photocatalytic performance of the Nb doped films to see if the high reactivity can be maintained in the visible range and optimization will look at the combined effects of cation doping and oxygen vacancy concentration.

Advances in Synergistic Polymer/Graphite and Polymer/Carbon Nanotube Nanocomposites and Sustainable Polymer Systems Using a Novel, Industrially Scalable Process Called Solid-State Shear Pulverization

John Torkelson,* Jun'ichi Masuda, Katsuyuki Wakabayashi, Cynthia Pierre, and Philip Brunner
Department of Chemical and Biological Engineering and Department of Materials Science and Engineering, Northwestern University

Solid-state shear pulverization (SSSP) is a novel, continuous process that involves a small modification to conventional twin-screw melt extrusion. Rather than heating the barrel in the apparatus, the barrel is cooled, resulting in the polymer samples being processed in the solid state. This means that the materials can experience greater shear stresses and compressive forces via SSSP than by conventional melt extrusion. Thus, relative to extrusion, SSSP can yield much superior dispersion of additives in a polymer matrix. We have taken advantage of this to produce polypropylene nanocomposites in which carbon nanotubes are dispersed as single nanotubes throughout the matrix and to achieve high levels of exfoliation of graphite in polypropylene. Relative to neat polypropylene, the resulting nanocomposites have yielded record enhancements of several mechanical properties as well as dramatic improvements in electrical conductivity. We have also applied SSSP to enhance the recyclability for high-value applications of a synthetic polymer, poly(ethylene terephthalate) (PET), and heat distortion temperature of poly(lactic acid) (PLA), a biobased, biodegradable polymer. The recyclability of PET is enhanced by taking advantage of mechanochemistry that can occur during SSSP, resulting in a transformation of linear PET to slightly branched PET with an enhancement in its melt-state viscosity. We have also increased the heat distortion temperature of PLA by incorporation and dispersion of 1 wt% microcrystalline cellulose into PLA during SSSP. The interfacial regions between the cellulose and PLA serve to strongly nucleate crystallization of PLA, meaning that after its is melt processed, the PLA made by incorporation of cellulose during SSSP exhibits much greater crystallinity (and a heat distortion temperature well above 400 K) than neat PLA (with a heat distortion temperature less than 333 K). Thus, the PLA/cellulose composites made by SSSP may be appropriate for use as hot beverage and food containers and provide a solution to new regulations in parts of Europe that will require all food waste (including containers) to be composted instead of being put in landfills.

Novel Green Light Emitting Diodes: Innovative Droop-free Lighting Solutions for a Sustainable Earth

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[a]Center for Quantum Devices, Department of Electrical Engineering and Computer Science, Northwestern University

[b]Nanovation SARL

Hybrid green light-emitting diodes (LEDs) comprised of *n*-ZnO/(InGaN/GaN) multi-quantum-wells/*p*-GaN were grown on semi-insulating AlN/sapphire using pulsed laser deposition for the *n*-ZnO and metal organic chemical vapor deposition for the other layers. X-ray diffraction revealed that high crystallographic quality was preserved after the *n*-ZnO growth. LEDs showed a turn-on voltage of 2.5 V and a room temperature electroluminescence (EL) centered at 510 nm. A blueshift and narrowing of the EL peak with increasing current was attributed to bandgap renormalization. The results indicate that hybrid LED structures could hold prospects for the development of green LEDs with superior performance. We discuss the current status of LEDs on non-/semi-polar planes, and propose an improved novel green LED that promise droop-free performance.

Separations of CO_2/CH_4 and CO_2/N_2 Mixtures Using Metal-Organic Frameworks

Youn-Sang Bae,[a] Omar K. Farha,[b] Karen L. Mulfort,[b] Alexander M. Spokoyny,[b] Chad A. Mirkin,[b] Joseph T. Hupp,[b] and Randall Q. Snurr[a]

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The separation of carbon dioxide from methane is an important process in natural gas upgrading because CO_2 reduces the energy content of natural gas and induces pipeline corrosion. The separation of carbon dioxide from nitrogen is needed for treatment of flue gas emissions from power plants (Flue gas: N_2 70%+, CO_2, water vapor, O_2, etc.) to capture the greenhouse gas CO_2. Compared to the conventional technologies for these separations, adsorption-based processes are attractive due to their low cost and high energy efficiency. High CO_2 selectivity and capacity are essential when selecting an adsorbent for a pressure-swing adsorption (PSA) process. Metal-organic frameworks (MOFs) are promising materials for gas separations due to tunable pores and functionalities, as well as well defined pores and exceptionally high surface area and porosity. This presentation will provide several strategies for improving the CO_2/CH_4 and CO_2/N_2 selectivities using MOF materials.

Solid State Lighting and Sensors

Chair: Siddhartha Ghosh, University of Illinois at Chicago

Tuesday, October 6, 1:00pm – 5:00pm

Brightness and Wavelength Dependence of Blue LEDs Upon Sapphire Off-cut Angle and Sapphire Patterning

Dr. Heinz Busta, Prairie Prototypes, LLC and University of Illinois at Chicago

Infrared Detectors

Mr. Koushik Banerjee, University of Illinois at Chicago

Confined Phonon Modes and Thermal Conductivity in Graphene

Mr. Jun Qian, University of Illinois at Chicago

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Patrick Shannon, Middough

Chair Novel Materials and Processing for Energy & Sustainability
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