ICOSSE'18

International Congress on
Sustainability Science & Engineering

AUGUST 12-15, 2018
CINCINNATI, OH

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The 7th International Congress on Sustainability Science & Engineering (ICOSSE '18) is organized by the AIChE Institute of Sustainability.

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Welcome Address

Dear Colleagues:

Welcome to Cincinnati and the 7th International Congress on Sustainability Science and Engineering (ICOSSE '18). This year's exciting program features speakers from leading companies, prominent universities, and various government entities. Together, they focus on industrial and environmental sustainability areas such as manufacturing, bioproducts, resilient socio-environmental systems, and the modeling approaches needed to better understand these systems. Through engaging with speakers and other participants, we hope you will leave ICOSSE '18 with an enriched outlook on the most current research and industry-oriented efforts in the field of sustainability science and engineering.

The 7th International Congress on Sustainability Science & Engineering serves as the international platform for innovation in sustainability science and engineering. Over the course of three days, the key themes – Food, Energy, Water, and the FEW Nexus; Industrial Innovation; Bioenergy Sustainability; and Modeling and Simulation – will be explored by oral and poster presentations and through ensuing discussions, in which we encourage you to take active part.

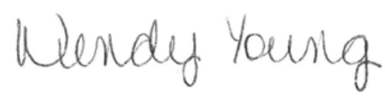
The plenary speakers at the beginning of each day will set the stage for the overarching themes of the Congress, which the keynote speakers and other presenters in the technical sessions that follow will explore in depth. Regular networking breaks will facilitate discussions between the speakers and audience. The Rapid Fire Session will introduce you to the work presented in the associated Poster Session, which plays a significant part in promoting the exchange of ideas at the Congress.

This conference would not be possible without the dedication and contributions from many of our colleagues. We acknowledge the efforts of our Steering Committee, input from the International Advisory Board, the leadership of the Session Chairs. We extend additional thanks to all of our invited and selected presenters, corporate sponsors, and academic and government supporters, without whom the conference would not be possible. Finally, we would like to thank you for coming and taking part in this conference and wish you a pleasant and enriching experience at ICOSSE '18!
Sincerely,

Conference Chairs

Raymond L. Smith
National Risk Management Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency

David Shonnard
Professor and Richard and Bonnie Robbins Chair
Department of Chemical Engineering
Director: Sustainable Futures Institute
Michigan Technological University



Wendy Young
AIChE Fellow
Business Development Manager
Chemstations Inc.

ICOSSE '18

International Congress on Sustainability Science & Engineering

INDUSTRY, INNOVATION AND SUSTAINABILITY

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ICOSSE '18: 7th International Congress on Sustainability Science and Engineering

Technical Program

Sunday, August 12, 2018

4:00 PM	**6:00 PM**	**Registration | Poster Setup**	
5:30 PM	**7:00 PM**	**Welcome Reception & Poster Display**	

Monday, August 13, 2018

7:00 AM	8:45 AM	Registration	
8:45 AM	**9:00 AM**	**Opening Ceremony**	
9:00 AM	**9:45 AM**	**Plenary Speaker: Oliver Kroner, Green Cincinnati Plan & Sustainability Coordinator, City of Cincinnati**	**Turning Science into Action: Sustainability Policy at the Ground Level**
9:45 AM	10:05 AM	Coffee Break	
10:05 AM	**10:50 AM**	**Keynote Speaker: Andrew Mangan, Business Council for Sustainable Development**	Transforming the Way Manufacturers Source, Value and Manage Materials
10:50 AM	**12:10 PM**	**Session 1 - Water and the Food-Energy-Water Nexus**	
		Session Chairs: Bhavik Bakshi, Ohio State University and Yinlun Huang, Wayne State University	
10:50 AM	**11:10 AM**	C. Stewart Slater, Rowan University	Integration of Membrane Technology into Coffee Manufacturing Operations for Water Recovery
11:10 AM	**11:30 AM**	Jason Trembly, Ohio University	Sustainable Management of Hypersaline Brine Waste: Zero Liquid Discharge Treatment of Produced Water Via Direct Joule-Heating Method
11:30 AM	**11:50 AM**	Nemi Vora, University of Pittsburgh	An Information Theory Approach to Assess U.S. Food Trade and Embodied Irrigation Impacts from a Food-Energy-Water Nexus Perspective
11:50 AM	**12:10 PM**	Irina Belozerova and Elizabeth Betancourt, Intel Corporation	Water Conservation in Semiconductor Industry: Ultrapure Water and Beyond
12:10 PM	1:30 PM	Lunch	
1:30 PM	**3:25 PM**	**Session 2 - Modeling and Simulation**	
		Session Chair: Wendy Young, Chemstations Inc.	
1:30 PM	**2:05 PM**	**Keynote Speaker: Heriberto Cabezas, U.S. Environmental Protection Agency and Pazmany Peter Catholic University**	Using Green Chemistry and Engineering Principles to Design, Assess, and Retrofit Chemical Processes for Sustainability
2:05 PM	**2:25 PM**	Fernando Lima, West Virginia University	A Simulation-Based Computational Framework for Pollution Control Units (PCU) and Estimation of Life Cycle Inventories (LCI) from Manufacturing Processes
2:25 PM	**2:45 PM**	Scott Nicholson, National Renewable Energy Laboratory	Assessing Fossil Fuel and Feedstock Use in the U.S. Plastics and Rubber Sector: A Supply Chain Analysis
2:45 PM	**3:05 PM**	Kirti M. Yenkie, Rowan University	Generating Efficient Wastewater Treatment Networks: An Integrated Approach Comprising of Contaminant Properties, Technology Suitability, Plant Design and Process Optimization
3:05 PM	**3:25 PM**	Andres Argoti, NRC Post-Doctoral Associate at U.S. Environmental Protection Agency	Assessment of Urban Sustainability of the Chicago Metropolitan Area Using Green Accounting Methods
3:25 PM	3:45 PM	Coffee Break	
3:45 PM	**4:30 PM**	**Rapid Fire Session**	
4:30 PM	**6:00 PM**	**Poster Session**	

Tuesday, August 14, 2018

7:30 AM	8:45 AM	Registration	
8:45 AM	**9:00 AM**	**Summary Session**	
9:00 AM	**9:45 AM**	**Plenary Speaker: Tracy Young, Global R&D Director, Construction Chemicals & Cellulosics Technology, The Dow Chemical Company**	**Building Better Solutions to Improve the World: How the Intersection of Technology and Sustainability are Key to Innovative Solutions for Tomorrow**
9:45 AM	10:05 AM	Coffee Break	
10:05 AM	**11:40 AM**	**Session 3 - Food-Energy-Water Nexus - Nutrient Considerations**	
		Session Chair: Heriberto Cabezas, U.S. Environmental Protection Agency and Pazmany Peter Catholic University	
10:05 AM	**10:40 AM**	**Keynote Speaker: Bhavik Bakshi, Ohio State University**	Accounting for Ecosystems Can Help Improve the FEW Nexus
10:40 AM	**11:00 AM**	Ranjani B. Theregowda, U.S. Environmental Protection Agency	Comparative Emergy Evaluation of Nutrient Recovery Technology as an Alternative to Traditional Fertilizers and Nutrient Removal Technologies
11:00 AM	**11:20 AM**	Briana Niblick, U.S. Environmental Protection Agency	Eutrophication Model Development for Life Cycle Impact Assessment in the United States
11:20 AM	**11:40 AM**	Xin Ma, U.S. Environmental Protection Agency	Nutrient Removal and Resource Recovery: Effect on Life Cycle Cost and Environmental Impacts of Small Scale Wastewater Treatment
11:40 AM	1:00 PM	Lunch	

1:00 PM	**2:55 PM**	**Session 4 - Bioenergy Sustainability**	
		Session Chair: Raymond Smith, U.S. Environmental Protection Agency	
1:00 PM	**1:35 PM**	**Keynote Speaker: Michael A. Schultz, PTI Global Solutions**	Drawing on the Past to Innovate Towards a Sustainable Future
1:35 PM	**1:55 PM**	Rebecca Hanes, National Renewable Energy Laboratory	Spatially Explicit Modeling of Criteria Air Pollutants from Agricultural and Forestry Feedstock Production
1:55 PM	**2:15 PM**	Wenqin Li, Iowa State University	Regional Techno-Economic (TEA) Analysis of the Pyrolysis-Bioenergy- Biochar Pathwayfor Carbon-Negative Energy
2:15 PM	**2:35 PM**	Eric C. D. Tan, National Renewable Energy Laboratory	An Integrated Sustainability Evaluation of Indirect Liquefaction of Biomass to Liquid Fuels
2:35 PM	**2:55 PM**	Jeffrey Seay, University of Kentucky Center for Applied Energy Research	Multi Objective Versus Single Objective Optimization of Batch Bioethanol Production Based on a Time-Dependent Fermentation Model
2:55 PM	3:15 PM	Coffee Break	
3:15 PM	**4:50 PM**	**Session 5 - Sustainable Bioproducts**	
		Session Chair: Rebecca Hanes, National Renewable Energy Laboratory	
3:15 PM	**3:50 PM**	**Keynote Speaker: Michael Gromacki, Dixie Chemical**	Upgrading of Glycerol, a Biodiesel By-Product, into a Speciality Epoxide, Glycidol, for Use in Coatings, Surfactants and Thermoset Materials
3:50 PM	**4:10 PM**	Bethany Klemetsrud, University of North Dakota	Aspects of Sustainable Production of Palm Oil in the Municipality of Teapa in Tabasco, Mexico: Evaluating the Current and Future Use of Palm Oil
4:10 PM	**4:30 PM**	Pahola Thathiana Benavides, Argonne National Laboratory	Life-Cycle Analysis of Bio-Derived Chemicals in the GREET Model
4:30 PM	**4:50 PM**	Alex Jordan, University of Pittsburgh	Dependence of United States Industrial Sectors on Pollination Service By Insects
4:50 PM	5:30 PM	Free Time	
5:30 PM	**6:00 PM**	**Awards Ceremony**	
6:00 PM	**8:00 PM**	**Sponsored Banquet**	

Wednesday, August 15, 2018

8:45 AM	8:55AM	Summary Session	
8:55AM	**9:40 AM**	**Plenary Speaker: Subhas Sikdar, U.S. Environmental Protection Agency (retired)**	**The Pursuit of Sustainable or Clean Products, Processes, and Network Systems**
9:40 AM	**11:15 AM**	**Session 6 - Sustainable Chemical Industry**	
		Session Chair: Gerardo Ruiz-Mercado, U.S. Environmental Protection Agency	
9:40 AM	**10:15 AM**	**Keynote Speaker: Emily Tipaldo, American Chemistry Council**	Plastic Industry Leadership in a Circular Economy: Ending Plastic Waste to the Environment
10:15 AM	**10:35 AM**	Paul F. Harten, U.S. Environmental Protection Agency	Program for Assisting the Replacement of Industrial Solvents, Paris III
10:35 AM	**10:55 AM**	Todd Martin, U.S. Environmental Protection Agency	Development of the Alternatives Assessment Dashboard
10:55 AM	**11:15 AM**	William M. Barrett, U.S. Environmental Protection Agency	Assessing Chemical Alternatives Based on Chemical Structure Using a Name Reaction Database
11:15 AM	**11:30 AM**	Coffee Break	
11:30 AM	**12:45 PM**	**Session 7 - Panel: Sustainability by Manufacturing USA Institutes**	
		Session Chair: David Shonnard, Michigan Technological University	
11:30 AM	**11:45 AM**	Ignasi Palou-Rivera, RAPID	Sustainability and Process Intensification
11:45 AM	**12:00 PM**	Nabil Nasr, REMADE	Remanufacturing & the Circular Economy
12:00 PM	**12:15 PM**	Haresh Malkani, CESMII	Sustainability and CESMII
12:15 PM	**12:45 PM**	Q&A/Discussion	
12:45 PM	**1:00 PM**	**Closing Remarks**	

~ ~ ~ End of ICOSSE '18 Programming ~ ~ ~

2:00 PM	4:00 PM	RAPID Workshop	

Thank you for attending ICOSSE ’17. We look forward to welcoming you to the next ICOSSE!
More information at www.icosse.org.

ICOSSE '18 Abstracts

PLENARY PRESENTATION – MONDAY

Monday, August 13, 2018
9:00 AM – 9:45 AM

Turning Science into Action: Sustainability Policy at the Ground Level.

Oliver Kroner
City of Cincinnati, Cincinnati, OH

How do we engineer cities to be more sustainable? Cities claim 2% of the earth, 54% of the human population, and over 70% of the world's carbon emissions. It has become increasingly clear that cities will lead the global effort to combat climate change. Cincinnati is on the frontlines, with a sustainability strategy that combines science, policy, technology, and behavior change to map the city's transition to a low-carbon economy.

KEYNOTE PRESENTATION

Monday, August 13, 2018
10:05 AM – 10:50 AM

Transforming the Way Manufacturers Source, Value and Manage Materials.

Andrew Mangan
Sustainable Development, Pathway 21, Austin, TX

Globally, more people are consuming more goods than ever before. This demand for natural resources, along with a widespread recognition that valuable materials are slipping into the waste stream, are among a set of factors driving companies and governments to embrace the idea of establishing a circular economy.

In the new global economy, reuse is standard, manufacturers get top value from all resources and nothing goes to landfill. Learn how companies and governments are joining forces to speed the shift to a circular economy by transforming the way manufacturers source, value and manage materials.

SESSION 1 - WATER AND THE FOOD-ENERGY-WATER NEXUS

Monday, August 13, 2018
10:50 AM – 12:10 PM
Session Chairs: Bhavik Bakshi, Ohio State University and Yinlun Huang, Wayne State University

Integration of Membrane Technology into Coffee Manufacturing Operations for Water Recovery.

C. Stewart Slater*, Mariano J. Savelski, and Christian Wisniewski*
Department of Chemical Engineering, Rowan University, Glassboro, NJ

Through a grant from the U. S. Environmental Protection Agency, we have partnered with Nestlé USA to explore water recovery in soluble coffee manufacture. A case study at their Freehold, NJ plant, has investigated water recovery methods to improve overall operational efficiency. The particular focus of this project is the study of a shear-enhanced vibratory field membrane method to recover water for reuse, and reduce fresh water consumption.

The food and beverage industry faces many challenges due to increasingly scarce and sustainable supplies of water for process operations. The production of spray and freeze-dried coffee involves many processes that rely on large amounts of water. These operations include process water for cooling, water to be heated to produce steam, water for process equipment operations, water for intermediate production steps, water for cleaning/sterilization, and water for operation of cooling towers.

Water recovery from waste streams is frequently hindered due to issues related to dissolved, colloidal, and particulate matter. These contribute to fouling and performance degradation in operating, as it is desired to produce sufficient quantity and quality of water for extended periods of time. Vibratory-field membrane processes provide a potential solution for efficient water recovery from food and beverage waste.

Our study evaluated the overall savings and reduction in life cycle emissions for the membrane-based recovery of water from a waste stream, for use in cooling tower operation. The assessment included savings, both economically and environmentally in the reduction in fresh water intake, waste pretreatment, and final disposal; which are compared to the increased cost and operational factors of a new recovery system. The case study found that the greatest cost and environmental impact reductions were associated with the reduction in wastewater discharge. Long-term economics were more highly influenced by capital equipment costs.

Sustainable Management of Hypersaline Brine Waste: Zero Liquid Discharge Treatment of Produced Water Via Direct Joule-Heating Method.

*Chad Able[1], David Ogden[2], and **Jason Trembly**[3]*
(1)Department of Chemical and Biomolecular Engineering, Ohio University, Athens, OH, (2)Chemical and Biomolecular Engineering, Institute for Sustainable Energy and the Environment, Athens, OH, (3)Institute for Sustainable Energy and the Environment, Ohio University, Athens, OH

Both U.S. energy and economic security rely upon continued development of U.S. unconventional shale plays, which require access to suitably clean water resources. Produced water (brine) is the nation’s largest industrial waste stream, with approximately 14 billion barrels generated annually by the U.S. oil and gas sector. The recent surge and continued development of unconventional U.S. shale plays will likely result in greater volumes of produced water. Utilizing this brine in development of unconventional shale resources represents a beneficial reuse of this waste stream. This approach can not only lower stress on local watersheds but can also address public/local government concerns regarding long-term ground water contamination potential and seismic activity associated with Class II salt water disposal wells (SWDs).

Ohio University (OHIO) with funding from the U.S. Department of Energy's National Energy Technology Laboratory (NETL) Crosscutting Research Program Project DE-FE0026315, has been developing an advanced supercritical water (SCW)-based process for treatment and beneficial reuse of brine waste streams. This SCW process offers an advantageous media for brine treatment, as its lower fluid density and decreased hydrogen bond strength provides a means to simultaneously remove dissolved solids and hydrocarbons.

To evaluate process potential, OHIO has been conducting both experimental investigations using prototype SCW reactors and process simulations/techno-economic assessments using Aspen Plus™. Removal of naturally occurring radioactive materials (NORM) using commercial ion exchange resins and natural adsorbent has been investigated. Further, removal of dissolved solids from simulated and field-derived produced water has been investigated at pressures ranging from 23-28 MPa, respectively, demonstrating the ability to recover greater than 99 percent of salts from brines containing dissolved solid concentrations greater than 240,000 $mg{\cdot}L^{-1}$. This presentation will present both experimental and process simulations findings from this study.

An Information Theory Approach to Assess U.S. Food Trade and Embodied Irrigation Impacts from a Food-Energy-Water Nexus Perspective.

Nemi Vora[1], *Brian D. Fath*[2], *and Vikas Khanna*[1]
(1)Civil and Environmental Engineering, University of Pittsburgh, Pittsburgh, PA, (2)Biological Sciences, Towson University, Towson, MD

We present a network model of the United States (U.S.) interstate food transfers, which we use to analyze the dependency of states with respect to participating regions and embodied irrigation impacts from a food-energy-water (FEW) nexus perspective. We compare whole system interactions of the food transfer network to understand mutual dependencies. To this end, we utilize the pointwise mutual information (PMI) measure to provide an indication of interdependencies by estimating probability of co-occurrences between state-trading dyads. Additionally, we compare observed trade flows with a null model of transfers (equitable trade) to assess presence of "additional information" in the system. The implications of PMI values are demonstrated by using Texas as an example, the largest importer in the US food transfer network. We find that Texas' neighbors Kansas, Oklahoma, Nebraska, and New Mexico demonstrate higher PMI values indicating a preference for trading with neighboring states. However, when considering irrigation water withdrawals, these states primarily rely on the highly depleted aquifers for irrigation, posing a risk for sustainable food supply for Texas. From an embodied GHG emissions perspective, we find that states with polluting emissions profile fare better for on-farm water applications, indicating hot-spots for irrigation pump upgrades by switching to less emissions-intensive fuels.

Water Conservation in Semiconductor Industry: Ultrapure Water and Beyond.

Irina Belozerova[1] *and* ***Elizabeth Betancourt***[2]
(1)Intel Corporation, Hillsboro, OR, (2)Intel Corporation, Chandler, AZ

Semiconductor industry has become one of the largest water consumers in the world. Semiconductor plant requires water for a variety of applications, however the majority of water is used to produce ultrapure water (UPW), critical to chemical processing of wafers. UPW is obtained by extensive treatment of city domestic water — removing virtually all contaminants, including bacteria, organic and inorganic compounds, dissolved gases, and particles. Of all high water-demanding manufacturing industries, including nuclear power, pharmaceutical, and textile, the semiconductor industry purity requirements are the most stringent, and its production is enabled by state-of-the-art technology.

The ever-increasing complexity and precision of computer chip manufacturing and consequent higher water quality standards introduce additional water treatment requirements, rejected impurities (and, with them, water), and equipment maintenance rinses. At a multi-thousand gallon-per-minute usage, it is essential to identify all opportunities for water saving both from sustainability and economical perspectives.

The market offers a variety of options for wastewater reclaim, as a conventional target area for semiconductor consumer. In addition, sufficiently clean water is rejected to wastewater collection systems along the UPW production process, which can be recovered without any treatment, once proper re-usage is identified. Even beyond UPW, every water conserving opportunity is thoughtfully considered, and evaluated for multifaceted returns on investment, regional water scarcities and industry benchmarking leadership.

Driven by ever-rising water costs and scarcity concerns, the semiconductor industry's approach to water conservation is comprehensive, searching for new opportunities to reclaim, reuse and recycle water while enabling technological progress.

SESSION 2 - MODELING AND SIMULATION

Monday, August 13, 2018
1:30 PM – 3:25 PM
Session Chair: Wendy Young, Chemstations Inc.

Keynote Presentation: Using Green Chemistry and Engineering Principles to Design, Assess, and Retrofit Chemical Processes for Sustainability.

Gerardo J. Ruiz-Mercado[1], *Ana Isabel Carvalho*[2], *and* ***Heriberto Cabezas***[1]
(1)Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH, (2)Engineering and Management, Instituto Superior Técnico, Lisbon, Portugal

The concepts of green chemistry and engineering (GC&E) have been promoted as an effective qualitative framework for developing more sustainable chemical syntheses, processes, and material management techniques. This has been demonstrated by many theoretical and practical cases. In addition, there are several approaches and frameworks focused on demonstrating that improvements were achieved through GC&E technologies. However, the application of these principles is not always straightforward. We propose using systematic frameworks and tools that help practitioners when deciding which principles can be applied, the levels of implementation, prospective of obtaining simultaneous improvements in all sustainability aspects, and ways to deal with multiobjective problems. Therefore, this contribution aims to provide a systematic combination of three different and complementary design tools for assisting designers in evaluating, developing, and improving chemical manufacturing and materials management systems under GC&E perspectives. The WAR Algorithm, GREENSCOPE, and SustainPro were employed for this synergistic approach of incorporating sustainability at early stages of process development. In this demonstration, simulated ammonia production is used as a case study to illustrate this advancement. Results show how to identify process design areas for improvements, key factors, multicriteria decision-making solutions, and optimal trade-offs. Finally, conclusions were presented regarding the tools' use in more robust sustainable process and material management designs.[1]

Disclaimer: The views expressed in this presentation are those of the author and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

[1] Ruiz-Mercado, G., Carvahlo, A, and H. Cabezas, "Using Green Chemistry and Engineering Principles to Design, Assess, and Retrofit Chemical Processes for Sustainability," ACS Sustainable Chem. Eng., 4 (11), 6208–6221 (2016).

A Simulation-Based Computational Framework for Pollution Control Units (PCU) and Estimation of Life Cycle Inventories (LCI) from Manufacturing Processes.

*Shuyun Li[1], Gerardo J. Ruiz-Mercado[2], and **Fernando V. Lima**[1]*
(1)Department of Chemical and Biomedical Engineering, West Virginia University, Morgantown, WV, (2)Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH

In the past, the chemical industry, as one of the primary stationary sources of air, liquid, and solid releases, has begun to shift from economic stand-alone focus to the inclusion of sustainability in the decision-making process. For example, LCI information, including release profiles, has been applied to chemical processes to analyze the process sustainability performance (Li, Ruiz-Mercado, and Lima et al., 2018). However, traditional chemical process design methods face challenges for incorporating LCI into the decision-making steps, such as: 1) limited capability of current process simulators in terms of available pollution control technologies; 2) lack of reliability in current LCI databases; and 3) difficult communication between process simulators and LCI tools.

In this work, it is proposed an integrated framework that involves process simulators and the development of parameterized PCU modules for waste treatment and LCI data generation. Specifically, the PCU modules with LCI capabilities are built using a user-friendly Microsoft Excel interface with the goal of facilitating its implementation by decision-makers with little process data or limited knowledge on specific waste treatment technologies. The proposed integrated framework with PCU and LCI augments the existing capacity of commercial process simulators (e.g., CHEMCAD). A user-friendly automation interface is built via Microsoft Excel-VBA to enable the communication between CHEMCAD and Excel PCUs and LCI generation tools.

The developed framework is applied to an acetic acid manufacturing process. Preliminary results show process improvements in terms of emissions represented by the LCI data after the implementation of the appropriate PCUs. The proposed framework can also be implemented for other decision-making applications, with the intent of facilitating the access to process design tools by other non-engineer practitioners.

The views expressed in this abstract are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

Assessing Fossil Fuel and Feedstock Use in the U.S. Plastics and Rubber Sector: A Supply Chain Analysis.

***Scott Nicholson**, Alberta Carpenter, and Rebecca Hanes*
Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO

In plastics and rubber manufacturing, fossil fuels are consumed both as an energy source and as feedstocks that are converted to higher-value products. For example, in the manufacture of polyethylene, natural gas is consumed both as a fuel and as a feedstock during ethylene production. In this work, we expand on the U.S. Department of Energy's Bandwidth Study on Energy Use and Potential Energy Savings Opportunities in U.S. Plastics and Rubber Manufacturing, which quantified onsite fuel consumption and the potential for reducing fuel consumption by increasing energy efficiency in the plastics and rubber sector. The bandwidth study did not quantify fuel consumed upstream in the supply chain or as a feedstock; however, both contribute significantly to a plastic's total fossil fuel requirements. The U.S. Energy Information Administration's 2014 Manufacturing Energy Consumption Survey (MECS) estimates that fossil fuels consumed as feedstocks account for approximately 74% of total fossil fuel consumption in the U.S. plastic resin manufacturing sector (NAICS 325211). We employ the Materials Flows through Industry (MFI) supply chain modeling tool, developed at the National Renewable Energy Laboratory (NREL), to quantify process fuel and feedstock requirements within the supply chains of the same 10 categories of plastics and rubber commodities covered in the DOE bandwidth report. From these results, we identify supply chains that will have a high feedstock requirement even when energy efficiency is increased. We then use MFI to analyze several alternative plastics supply chains, including those utilizing biomass feedstocks and/or polyethylene terephthalate (PET) waste upcycling, to determine if these alternatives can potentially reduce both process fuel and feedstock requirements within the supply chains of interest. This presentation will include a case study comparison of supply chain energy consumption for petroleum-derived and bio-derived fiberglass reinforced plastic involving a novel waste PET upcycling technique recently discovered by NREL researchers.

Generating Efficient Wastewater Treatment Networks: *An Integrated Approach Comprising of Contaminant Properties, Technology Suitability, Plant Design and Process Optimization*.

James Dailey, Sean Burnham, and ***Kirti M. Yenkie***
Chemical Engineering, Rowan University, Glassboro, NJ

The rise in world population and industrialization in developing nations has tremendously increased the demand for water and has resulted in wastewater contaminated with several pollutants. Thus, wastewater treatment, reuse, and safe disposal have become crucial for sustainable existence. Systematic guidelines which propose treatment based on inlet contamination and final desired conditions for water reuse and safe disposal can aid in designing efficient wastewater treatment and management systems. The treatment methods must vary based on the properties of the wastewater stream entering a treatment plant, such as: number of contaminants, their amounts, toxicity, shape, size, etc. To this end, a superstructure comprising of all possible treatment methods and an optimization strategy that eliminates certain technology options based on cost, and specific physical constraints, will make the generation of wastewater treatment networks more efficient. The technologies involved in wastewater treatment such as sedimentation, filtration, membranes, disinfection, adsorption, and activated sludge are modeled using the material and energy balance, equipment design, costing as well as environmental impact, which is in the form of linear and non-linear mathematical models. After model generation, the individual models are combined into the superstructure to create an optimization model where the technology selection is represented by integer constraints. The overall wastewater treatment process is optimized for cost using mixed integer non-linear programming (MINLP) solvers in GAMS (General Algebraic Modeling Systems).

In our analysis, we demonstrate two case studies: (i) treatment of municipal wastewater for reuse for cropland irrigation and (ii) treatment of pharmaceutical effluent by including additional technologies such as UV/H_2O_2 oxidation processes and specialized biological membranes. These case studies are examined to meet the regulations specified by the 1972 Clean Water Act and the title 40 regulations for pharmaceutical effluents specified by the US EPA.

Assessment of Urban Sustainability of the Chicago Metropolitan Area Using Green Accounting Methods.

Bayou Demeke and ***Andres Argoti***
Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH

Herein, we assess the sustainability trend of the Chicago Metropolitan Area (CMA) by means of metrics rooted in economics, which follow a green accounting methodology. Specifically, we deploy the Green Net Metropolitan Product (GNMP) and Genuine Savings (GS). GNMP adjusts the Gross Metropolitan Product by subtracting the value of consumption of physical capital, the costs associated with depletion of natural resources, and the costs of damages associated with environmental pollution. GS measures changes in total capital stock (wealth), including man-made capital, human capital, and natural capital. Commonly applied conditions for sustainable development are the ability of a given region to maintain non-declining utility over time (i.e. non-declining GNMP) or to maintain non-declining wealth over time (i.e. non-negative GS). We estimate the CMA's GNMP and GS for the period, 1990-2015, by using economic and environmental data for the counties in the region. These data have been collected from various public outlets, including the Chicago Metropolitan Agency for Planning (CMAP) and USEPA. In estimating the CMA's GNMP and GS, we have accounted for the damage costs associated with air emissions based on marginal damage cost estimates from the literature via the benefit transfers method as described in Demeke et al. (2018), Heberling et al. (2012), Wu and Heberling (2016). Moreover, we also attempt at accounting for the marginal value of depletion of natural resources in the CMA in terms of water depletion, changes in urban ecosystem services, and the marginal damage cost of solid waste. In addition, we also incorporate the value of time to account for technological change. We expect that the methods and results of this study will assist CMAP planners in incorporating integrated metrics for the planning of regional sustainability.

PLENARY PRESENTATION – TUESDAY

Tuesday, August 14, 2018
9:00 AM – 9:45 AM

Building Better Solutions to Improve the World: How the Intersection of Technology and Sustainability are Key to Innovative Solutions for Tomorrow.

Tracy Young
Construction Chemicals & Cellulosics Technology, The Dow Chemical Company, Midland, MI

With the world population estimated to reach 8.3 billion by 2030, global demand is expected to increase 30% for water, 45% for energy, and 50% for food. The world is also undergoing the largest wave of urban growth in history with a projected 67% of our population to live in urban cities by 2030. Designing breakthrough solutions to these challenges is the next intersection of innovation for the future to bring together technology, sustainability, and new business model system approaches. As researchers, we play a key role in bringing science to the fore-front to ensure innovations and economic solutions are adopted to meet the needs of our world tomorrow. In this talk, I will highlight some of the development history for the circular economy goal in water and global innovation challenges across the Construction and Infrastructure market.

ICOSSE '18 Abstracts

SESSION 3- FOOD-ENERGY-WATER NEXUS - NUTRIENT CONSIDERATIONS

Tuesday, August 14, 2018
10:05 AM – 11:40 AM
Session Chair: Heriberto Cabezas, U.S. Environmental Protection Agency and Pazmany Peter Catholic University

Keynote Presentation: Accounting for Ecosystems Can Help Improve the FEW Nexus.

Bhavik R. Bakshi
William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH

Most approaches for assessing sustainability and understanding the food-energy-water nexus tend to focus on human activities such as manufacturing, farming, and consumption. This is in parallel with the dominant paradigm in most disciplines that takes nature for granted or greatly undervalues its role. Even methods for sustainability assessment such as life cycle analysis do not account for the capacity of ecosystems to supply the goods and services that are essential for sustaining the activities being assessed. Such approaches aim to reduce environmental impacts without considering the capacity of nature to absorb the impact. Keeping nature outside the system boundary can result in decisions that cause unintended harm by increasing reliance on degraded ecosystems, and lost opportunities for discovering innovative solutions that may be economically and environmentally superior. The framework of techno-ecological synergy aims to overcome these shortcomings of existing methods. This talk will consider the food-energy-water nexus of agricultural and land use practices with and without accounting for the role of relevant ecosystems. By application to a typical landscape in Ohio, this work will show how the trade-off between food production, water quality, greenhouse gas emissions, and net present value can be enhanced due to the free services provided by nature. Opportunities for further work with spatially explicit models will also be described.

Comparative Emergy Evaluation of Nutrient Recovery Technology as an Alternative to Traditional Fertilizers and Nutrient Removal Technologies.

Ranjani B. Theregowda[1]*, Alejandra González-Mejía*[2]*, Xin Ma*[3]*, and Jay Garland*[4]
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Nitrogen (N) and phosphorus (P) nutrient discharge regulations are becoming more stringent with increased environmental impacts, especially in surface water bodies. Many wastewater treatment plants (WWTPs) have been equipped with the necessary nutrient removal technologies to meet their effluent discharge permits. Though these processes can remove nutrients to very low levels, the treatment costs rise tremendously, burdening WWTPs and rate-payers for capacity expansion, increased capital investment and operational expenditure.

In the past decade, nutrient recovery technologies have demonstrated potential benefits in recovering nitrogen and phosphorus from wastewater as fertilizers. These recovery technologies not only fulfill the long-term goals of compliance with nutrient discharge limits but also provide WWTPs with a revenue source, that can alleviate the resource scarcity associated with the depletion of P reserves and improve sustainability and resilience of the communities. Thus, to develop sustainable water systems integrated with ecosystems services (i.e., phosphorous reserves), this research evaluates fertilizer production from struvite (i.e., magnesium ammonium phosphate hexahydrate) that is generated from domestic wastewater and compares it with traditional commercial fertilizers (e.g., diammonium phosphate). Further, this study compares different levels of nutrient removal (chemical addition with - Modified Ludzack-Ettinger or Bardenpho or Modified University of Cape Town Processes with added Filtration or Osmosis) by using emergy as a sustainability metric. Emergy is used to provide system analysis including energy use, nutrient/eutrophication reduction, revenue stream, and whole system efficiency. The study will provide insights into 1) how regulations drive the system changes, and 2) how the conventional system can be transitioned to more cost-effective and sustainable alternatives in nutrient management.

Eutrophication Model Development for Life Cycle Impact Assessment in the United States.

Briana Niblick[1], *Ben Morelli*[2], *Troy R. Hawkins*[3], *Andrew Henderson*[4], *Heather Golden*[5], *Jana Compton*[6], *Ellen Cooter*[7], *and Jane Bare*[1]
(1)National Risk Management Research Laboratory, U.S. Environmental Protection Agency, Cincinnati, OH, (2)Eastern Research Group, Inc. (ERG), Lexington, MA, (3)Eastern Research Group, Inc. (ERG), Cincinnati, OH, (4)Noblis, Inc., San Antonio, TX, (5)National Exposure Research Laboratory, U.S. Environmental Protection Agency, Cincinnati, OH, (6)National Health and Environmental Effects Research Laboratory, U.S. Environmental Protection Agency, Corvallis, OR, (7)National Exposure Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC

Eutrophication describes the buildup of excess nutrients, such as nitrogen and phosphorus, in a body of water. This buildup can lead to excess plant growth, such as harmful algal blooms (HABs), resulting in deficiency of dissolved oxygen (hypoxia), and in some cases the production of cyanotoxins. Life cycle assessment (LCA) can evaluate Eutrophication Potential (EP) over the life cycle of a product or service, but the way EP is calculated depends on the particular life cycle impact assessment (LCIA) method used. Different methods rely on different fate and transport (F&T) models, which when paired together with varying user assumptions, can lead to vastly different results.

Commonly used approaches to EP are currently most appropriate for screening-level analyses. The necessary simplification of F&T models, particularly with regard to spatial and temporal scopes, can make it difficult to inform eutrophication-based life-cycle decisions without including significant levels of uncertainty. Yet such decisions need to be made and these decisions have far-reaching effects on water quality, nutrient management, and environmental policies.

This presentation builds on a critical review of nutrient F&T models (e.g. NEWS 2, WASP, AQUATOX) as well as eutrophication LCIA methods (e.g. TRACI, ReCiPe, IMPACT World+) and offers recommendations on how the EP impact category could be improved to better inform life-cycle decision-making, especially in the United States. These recommendations extend to EPA's update of the Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI) and ongoing methodology research for other impact categories at EPA.

The views expressed in this abstract are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Nutrient Removal and Resource Recovery: Effect on Life Cycle Cost and Environmental Impacts of Small Scale Wastewater Treatment.

Ben Morelli[1], Sarah Cashman[1], ***Xin Ma[2]****, Jay Garland[3], Jason Turgeon[4], Lauren Fillmore[5], and Diana Bless[6]*
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Many municipalities are facing the call to increase nutrient removal performance of their wastewater treatment plants in order to limit the impacts of eutrophication on the receiving waterbodies. The associated upgrades often demand investment in new technologies and increases in energy and chemical use, which create the potential for environmental trade-offs. The main goal of this study is to quantify these trade-offs for Bath NY wastewater treatment plant (WWTP) from an environmental and cost perspective by performing a life cycle assessment and cost analysis. The impacts of a conventional activated sludge treatment process are compared against an upgraded system incorporating chemically enhanced primary settling, Modified Ludzack-Ettinger secondary treatment, and anaerobic digestion (AD). The sensitivity analysis explores the effect of composting emission assumptions, AD operational performance, and the use of excess AD capacity for the processing of high strength organic waste on environmental impact and cost per cubic meter of wastewater treated.

The results generally show that improvements in environmental performance are available to communities that undertake a similar approach to treatment plant upgrades. Improved environmental performance is largely due to the inclusion of AD, and the avoided electricity and heat production that is a result of energy recovery from biogas. This study revealed that plant level impact scores are sensitive to AD operational performance and greenhouse gas emissions associated with composting, indicating the importance of sound management of these unit processes if improvements are to be realized across environmental impact categories. This study shed some light on how to retrofit existing WWTPs for compliance needs and the balance of compliance and sustainability.

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SESSION 4 - BIOENERGY SUSTAINABILITY

Tuesday, August 14, 2018
1:00 PM – 2:55 PM
Session Chair: Raymond Smith, U.S. Environmental Protection Agency

Keynote Presentation: Drawing on the Past to Innovate Towards a Sustainable Future.

Michael A. Schultz
PTI Global Solutions, Glen Ellyn, IL

Drake's historic Titusville well produced 20 barrels a day in 1859. Innovation along the entire supply chain grew over time to enable the offshore wells that today produce up to 250,000 barrels per day, and refineries that convert more than 1 million barrels per day. Certainly, the scale of today would have seemed impossible to those working in Titusville in 1859. Technology development played a significant role in this 10,000X increase in scale, as larger equipment became standard rather than first of its kind, process optimization, operational procedures, and supply chain development continued to drive down the cost of production, and operational experience informed process design methods that enabled further technology innovation.

These process design methods provide a template that can be adapted to the design of industrial biotechnology processes. Industrial biotechnology has been practiced for decades, if not centuries, and in more recent times has been implemented as an approach to reduce reliance on petroleum derived fuel and chemical products. While the challenges associated with industrial biotechnology may be different than those of conventional hydrocarbon processing, the same process design methods can be adapted in areas such as:

- Kinetic modeling of the biological system
- Reactor selection and design
- Cell and metabolite recovery

This presentation will present examples of these design challenges, and the hydrocarbon process design methods that can be adapted to continue to push the boundaries of what is possible in the drive towards a sustainable future.

Spatially Explicit Modeling of Criteria Air Pollutants from Agricultural and Forestry Feedstock Production.

***Rebecca Hanes**, Yimin Zhang, Daniel Inman, Annika Eberle, Garvin Heath, and Dylan Hettinger*
Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO

The Feedstock Production Emissions to Air Model (FPEAM) is a spatially explicit supply chain model that quantifies criteria air pollutants and precursors generated by biomass production, harvest and transportation to biorefineries. FPEAM was most recently used for the 2016 Billion Ton Study (BTS) published by the U.S. Department of Energy Bioenergy Technologies Office.

This presentation describes several use cases for the model, and provides an overview of recent restructuring that increases FPEAM's usability and functionality.

FPEAM currently estimates emissions of volatile organic compounds, particulate matter, nitrogen oxides, sulfur oxides, and carbon monoxide from on-farm equipment operation, on-farm fugitive dust, on-farm chemical (fertilizer, herbicide and insecticide) application, and biomass transportation. These calculations are implemented within FPEAM as modules, which independently perform calculations for each emissions category. This structure allows users to include or exclude emissions categories according to the goal and scope of their analysis. Each module's input data defines the activities taking place with information including fuel combusted, chemicals applied, and equipment used.

Users can replace or augment the default input data to quantify additional pollutant types, emissions categories, farming practices and biomass types. Emissions from biomass transportation and on-farm equipment operation are by default calculated by the U.S. Environmental Protection Agency's Motor Vehicle Emission Simulator (MOVES) and NONROAD model, respectively. These models – which are computationally intensive but provide detailed results – can optionally be replaced with user-provided emissions factors for fuel combustion and vehicle operation. This approach reduces FPEAM's runtime and allows users to run sensitivity analyses around biomass production and transportation scenarios.

Other enhancements currently under development are the use of farm-to-biorefinery route information to increase the spatial resolution of transportation emissions, and a module to connect FPEAM and the Intervention Model for Air Pollution (InMAP), which will enable the quantification of human health impacts.

Regional Techno-Economic (TEA) Analysis of the Pyrolysis-Bioenergy- Biochar Pathwayfor Carbon-Negative Energy.

Wenqin Li[1]*, Mark Mba Wright*[2]*, Robert C. Brown*[3]*, David Laird*[1]*, Hamze Dokoohaki*[1]*, Fernando E. Miguez*[1]*, and Jerome Dumortier*[4]
(1) Iowa State University, Ames, IA, (2)Mechanical Engineering, Iowa State University, Ames, IA, (3)Bioeconomy Institute, Iowa State University, Ames, IA, (4)Indiana University–Purdue University Indianapolis, Indianapolis, IN

The objective of this project is to evaluate regional economic impacts of an integrated pyrolysis-bioenergy-biochar industry to produce carbon negative energy. Utilization of biochar co-produced from fast pyrolysis process as soil amendment is essential to produce carbon negative energy. Selection of the pyrolysis biorefinery location is important since it involves feedstock availability and prices, biochar demand and credits, soil type and quality, and logistics etc. Therefore, we conducted an economic analysis including regional factors to determine the best biorefinery location to maximize the economic benefits of the pyrolysis-bioenergy-biochar platform.

Three specific land areas of US are investigated depending on the selection of pyrolysis facility locations: Upper Mississippi River Basin (UMRB), U.S. Southeast and California. Three counties including Hamilton (Iowa), Jackson (Florida) and Glenn (California) were selected to represent these three regions. We applied biochar produced from fast pyrolysis of corn stover, switchgrass and forest residue to crop lands for corn, peanuts and rice individually for these three counties. The correlation between biochar application to crop yields change were modeled based on over 100 previous literatures. The mean crop yield increases have been predicted as 2.9%, 10% and 4.5% in Hamilton, Jackson and Glenn. The biochar prices that the farmers are willing to pay were calculated as $113, $475 and $262 per metric ton with a biochar application rate of 5 metric tons per hectare.

Capital costs are also sensitive to the biorefinery location. The location multipliers have been suggested as 0.92, 0.82 and 1.17 for Iowa, Florida and California in Dodge unit cost guide. The feedstock costs vary with the feedstock type in different regions. The capital cost, operating cost and minimum fuel selling price were estimated over three different states to identify the most economic beneficial location to build this pyrolysis-biochar-bioenergy platform.

An Integrated Sustainability Evaluation of Indirect Liquefaction of Biomass to Liquid Fuels.

Eric C. D. Tan *and Mary Biddy*
National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO

Developing a more sustainable biofuel production process holds the key for displacing fossil fuels with biofuels for sustainable greenhouse gas emissions and natural resource consumption mitigation. A holistic sustainability analysis for the production of biofuel plays a critical role on the improvement of the overall life cycle sustainability. Once a conceptual conversion process is developed, the next step is to evaluate its overall sustainability, preferably based on a process sustainability evaluation methodology using various indicators. The EPA's GREENSCOPE methodology evaluates processes in four areas: environment, energy, economics, and efficiency. The method develops relative scores for indicators that allow comparisons across various technologies. In this study, we have implemented GREENSCOPE methodology for a sustainability performance assessment of NREL's indirect liquefaction of biomass to high-octane gasoline blendstock by evaluating a range of metrics beyond the typical minimum fuel selling price and greenhouse gas considerations. We applied this methodology to evaluate the sustainability performance of this gate-to-gate conceptual design. One outcome of the sustainability evaluation is to allow researchers to identify process areas in need of sustainability improvement, as well as the challenges and opportunities for achieving the best possible sustainability target.

Multi Objective Versus Single Objective Optimization of Batch Bioethanol Production Based on a Time-Dependent Fermentation Model.

Kwabena Darkwah[1], Barbara L. Knutson[2], and ***Jeffrey Seay[3]***
(1)University of Kentucky Center for Applied Energy Research, Lexington, KY, (2)Department of

Chemical and Materials Engineering, University of Kentucky, Lexington, KY, (3)Chemical and Materials Engineering, University of Kentucky, Paducah, KY

Microorganisms used in fermentation are susceptible to both substrate and product inhibitions. This results in dilute aqueous fermentation broths with consequential significant downstream separation costs. This work uses time-dependent information from Aspen Plus coupled with the robust multi-objective (MOO) and single-objective (SOO) genetic algorithm optimizations in MATLAB to design and optimize batch fermentation and integrated batch and *in situ* product separation with respect to initial substrate concentration, fermentation time and *in situ* product removal conditions of gas flow rate and gas stripping initiation times. The crippling effect of substrate and product inhibitions on fermentation process will be demonstrated using the time-dependent information. Unlike the single optimal solution from the SOO, MOO presents many equally optimal solutions that can be used to reveal the trade-off and interactions among competing process objectives and as a decision-support tool to guide the choice of design variables and conditions for optimum process performance.

SESSION 5 - SUSTAINABLE BIOPRODUCTS

Tuesday, August 14, 2018
3:15 PM – 4:50 PM
Session Chair: Rebecca Hanes, National Renewable Energy Laboratory

Keynote Presentation: Upgrading of Glycerol, a Biodiesel By-Product, into Specialty Epoxide, Glycidol, for Use in Coatings, Surfactants and Thermoset Materials.

Michael Gromacki[1]*, Alex Grous*[2]*, Fergal Coleman*[3]*, and Martin Atkins*[4]
(1)Dixie Chemical, Houston, TX, (2)Dixie Chemical, Houston, (3)Green Lizard Technologies, Teeside, United Kingdom, (4)Green Lizard Technologies, Belfast, United Kingdom

Glycidol, or 2,3-epoxy-1-propanol is a specialty epoxide that contains both epoxide and 1° alcohol functionalities. Due to this combination of functionality, glycidol is a versatile chemical building block with many diverse industrial applications, including in surfactants, coatings, thermosets and in the synthesis of chemical intermediates. However, its wider uptake in a range of high volume applications has been hindered by its high cost.

Commercially, glycidol is produced by 2 main routes; epoxidation of allyl alcohol and epichlorohydrin hydrolysis/dehydrodechlorination. These processes are not without drawbacks, generating large amounts of waste by-products. Unfavourable reagents, including peroxide oxidants and HCl/Cl2 gas are used in these processes or in starting materials production. Furthermore, epichochlorohydrin and allyl alcohol are derived from propylene, a non-renewable feedstock. The combination of these factors results in a high EP cost of production.

Dixie Chemicals, together with partners Green Lizard Technologies (UK) and Felda Global Ventures (Malaysia), have developed an innovative and economically attractive process for the production of glycidol from glycerol carbonate which is easily synthesized from biodiesel byproduct, glycerol. The patented process, currently at pilot scale (50 kg/day), utilizes a thin film evaporator as the main reactor which allows efficient evaporation of the produced glycidol, thereby minimizing its polymerization.

Working with Process Design Centre (NL) we have completed a full conceptual process design and techno-economic analysis for a 10 KTPA plant. Arising from this, the total production cost for glycidol is expected to be a fraction of the current market price. Glycidol has a growing market opportunity in the replacement of ethylene oxide and epichlorohydrin for a number of processes, particularly in the manufacture of glycidyl methacrylate, CO_2 capture solvents and non-ionic surfactants. In addition, the byproduct polyglycerols find application in polyurethanes & polyesters production, as polymer additives and food additives, as demulsifiers and in drilling fluid formulations.

Aspects of Sustainable Production of Palm Oil in the Municipality of Teapa in Tabasco, Mexico: Evaluating the Current and Future Use of Palm Oil.

Bethany Klemetsrud[1]*, Carlos García*[2]*, Cesar J. Vazquez-Navarrete*[3]*, Jessie Knowlton*[4]*, Colin Phifer*[5]*, Ena Mata Zayas*[6]*, Amarella Eastmond*[7]*, Erin Pischke*[8]*, and David R. Shonnard*[9]
(1)Chemical Engineering, University of North Dakota, Grand Forks, ND, (2)Environmental Sciences, Escuela Nacional de Estudios Superiores Unidad Morelia-UNAM, Morelia, Mexico, (3)Ciencia de los alimentos e ingeniería, Colegio de Postgraduados, Tabasco, Mexico, (4)School of Forest Resources and Environmental Science, Michigan Technological University, Houghton, MI, (5)School of Forest Resources and Environmental Sciences, Michigan Technological University, Houghton, MI, (6)Universidad Juarez Autonoma de Tabasco, Villahermosa, Mexico, (7)Unidad de Ciencias Sociales, Universidad Autonoma de Yucatan, Merida Yucatan, Mexico, (8)Social Sciences, Michigan Technological University, Houghton, MI, (9)Chemical Engineering, Michigan Technological University, Houghton, MI

Palm has been considered an advantageous food and bioenergy crop, due to its high fruit yields and high oil content, approximately 40% by mass. Currently in the municipality of Teapa in the state of Tabasco, Mexico several palm plantations exist and are being expanded to accommodate the growing demand for vegetable oil markets and potential biodiesel markets. This study site evaluates several different aspects of sustainability when considering palm as a current food crop along with the future use as a feedstock for biodiesel. Social, economic and environmental indicators were used to evaluate the multidimensional understanding of sustainability. 55 palm plantations were evaluated and the data aggregated to evaluate the overall sustainability of palm cultivation. Data such as soil C, wild pollinator count, fertilizers and insecticides use, palm fruit yield, etc., were collected from a questionnaire of local plantation owners along with measurements from field ecologists. A life cycle assessment (LCA) was conducted to evaluate overall greenhouse gas emissions, water consumption and air quality of the current production along with the future use of palm as a renewable energy feedstock. The LCA includes direct soil C land use change, land preparation, fruit harvest and transportation and oil extraction when evaluating the current use of palm oil. When looking to future use, the LCA includes processing of the palm oil into biodiesel and final combustion

within vehicles. Socioeconomic conditions were evaluated within the state of Tabasco to look at social and economic impacts of expanded palm production for palm oil and/or palm biodiesel. Indicators such as working conditions, income, and employment were evaluated within the current use of the palm oil and were extrapolated to evaluate future production of palm biodiesel. This study takes a multidimensional approach to sustainability and recommends best practices for the continued expansion of palm oil production.

Life-Cycle Analysis of Bio-Derived Chemicals in the GREET Model.

Pahola Thathiana Benavides[1] *and Hao Cai*[2]
(1)Energy System, Argonne National Laboratory, Chicago, IL, (2)Energy Systems Division, Argonne National Laboratory, Argonne, IL

Bio-derived chemicals play an important role in promoting bioeconomy. They provide great opportunity to boost the U.S. chemical industry while improving the sustainability of integrated biomanufacturing, reducing U.S dependence on fossil-derived sources, and encouraging creation of new domestic bioproduct industry. Under the bioenergy technologies office (BETO) founded programs like ABF (Agile BioFoundry) new pathways have been studied to produce desired products such as advance biofuels, fuel intermediates and bioproducts. ABF is integrating advanced computational tools for biological engineering, process design and data analysis, techno-economic and life-cycle analysis into an agile and dynamic platform for biomanufacturing of microbes (hosts) and using them in the production of bio-based fuels and chemicals. Life-cycle analysis can be very helpful to identify opportunities to improve the environmental footprint of bioproducts, especially while products are still in research and development (i.e. early stage of technology). Conducting environmental analysis of bioproducts at the early-stage will allow scientist, designers, and engineers to improve the production processes for sustainability. We present how we are expanding the GREET (Greenhouse gases, Regulated Emissions, and Energy use in Transportation) model, famously known for the evaluation of environmental impacts of advanced vehicle technologies and alternative transportation fuels, to assess environmental impact of new bio-derived chemicals produced from biochemical, biological, and thermochemical conversion technologies. We conduct LCA on three target/host bioproducts choose under the ABF program: acrylic acid using aspergillus pseudorerreus as the host, adipic acid via beta-ketoadipate using pseudomonas putida, monoterpenoid (1, 8 cineole) using rhodosporidium toruloides. We also evaluate the key drivers of the GHG emissions and water consumption. These biomass-derived chemicals can displace fossil-derived products and reduce GHG emissions and fossil fuel consumption as compared to their fossil-derived counterparts.

Dependence of United States Industrial Sectors on Pollination Service By Insects.

Alex Jordan[1]*, Margaret Douglas*[2]*, Harland Patch*[3]*, Christina Grozinger*[3]*, and Vikas Khanna*[1]
(1)Civil and Environmental Engineering, University of Pittsburgh, Pittsburgh, PA, (2)Dickinson College, Carlisle, PA, (3)Pennsylvania State University, State College, PA

Of the many goods and services provided by ecosystems that are crucial to humans and their industries, one critical service with high economic value is pollination by insects. A lack of this service would be a significant detriment to ecosystem biodiversity and function, but also to human nutrition and the United States national economy. Agricultural sectors and related sectors *(fiber, drugs, and fuel)* are directly and indirectly dependent on insect-mediated pollination by both commercially-managed species and wild species of bees and other insects. Production of pollination-dependent crops has increased at a faster rate (50-62%) than the global population of managed bees (45%) as many stress factors influence the fitness of pollinators around the world. In addition, the abundance and biodiversity of wild insects suffer in all regions, including natural protection areas. This disparity between production demand and pollinator supply is a concern nutritionally as well as economically, especially in Europe and North America which are particularly vulnerable as pollinator stocks in these regions decline.

Using field study data on pollination of specific crops available in the literature, we quantify economic dependence of crops in the United States on pollination services by insects, updating existing coefficients of dependence when possible, bounding uncertainty of estimates, and limiting the scope to U.S. landscapes. Data compiled at a national, state, and county level, considers the spatial relationship between the economic value of pollination, region-specific pollinator forage suitability, and crop-specific agricultural areas. Price and production data integration reveal areas of the U.S. which are highly dependent on pollination service by insects as well as those areas most vulnerable to decline. The implications of these findings include directing conservation and suitable forage revitalization efforts, advising future policy development, and supporting the incorporation of valuable ecosystem goods and services as a component of life cycle assessment.

PLENARY PRESENTATION - WEDNESDAY

Wednesday, August 15, 2018
8:55 AM – 9:40 AM

The Pursuit of Sustainable or Clean Products, Processes, and Network Systems.

Subhas Sikdar
National Risk Management Research Lab, US EPA, Cincinnati, OH

The adjective "sustainable" before products, processes or system networks is subjective, since we cannot define a benchmark for sustainability of any chosen system at any scale. The word "sustainability" has been applied to resources such as energy and water, to products, processes, urban infrastructure, or a quasi-natural infrastructure such as an eco-system. Implied in all analyses of sustainability is quantification of incremental betterment from economic, environmental and societal impacts perspectives. Attempts have been made to integrate the impacts of these three sustainability domains with offerings of "sustainability index" but their penetration in industrial practice so far has been marginal, for various reasons. Claims of industrial sustainability are limited to citations of emissions and discharge reductions and material and energy usage. This discussion is largely dominated these days by the emission reduction of greenhouse gases, chiefly carbon dioxide. Yet, from an industrial perspective, such a limited sustainability assertion may be reasonable, given the cost of detailed analyses and their inherent uncertainty. This presentation will examine the issues over which we must have better control in order to promote cleaner or greener products and processes.

SESSION 6 - SUSTAINABLE CHEMICAL INDUSTRY

Wednesday, August 15, 2018
9:40 AM – 11:15 AM
Session Chair: Gerardo Ruiz-Mercado, U.S. Environmental Protection Agency

Keynote Presentation: Plastic Industry Leadership in a Circular Economy: Ending Plastic Waste to the Environment.

Emily Tipaldo
American Chemistry Council Plastics Division, Washington, DC

The plastics industry is embracing the drive toward a circular economy. Together with our value chain partners the industry intends to transition to increasingly circular systems for designing, manufacturing, recycling and recovering our plastic packaging resources. Specifically, to achieve our goals, plastic resin producers plan to focus on six key areas: designing new products for greater efficiency, recycling and reuse; developing new technologies and systems for collecting, sorting, recycling and recovering materials; making it easier for more consumers to participate in recycling and recovery programs; expanding the types of plastics collected and repurposed; aligning products with key end markets; and expanding awareness that used plastics are valuable resources awaiting their next use.

Program for Assisting the Replacement of Industrial Solvents, Paris III.

Paul F. Harten
ORD/NRMRL/LMMD, US EPA, Cincinnati, OH

PARIS III is a solvent substitution software tool freely downloaded from the US Environmental Protection Agency. It finds chemical mixtures that have physical and chemical properties very similar to current industrial solvents, but are significantly less harmful to the environment. By using common laptops and workstations, extensive searches through the millions of combinations of chemical mixtures necessary can be completed. These searches may be refined and performed repeatedly by changing how close certain properties of the replacement solvents should be to those of the original solvent, and by adjusting how important different types of environmental impacts are. This software tool provides an effective and user-friendly way of finding greener replacements for harmful solvents used by industry; and it may be implemented by environmental engineers, chemical engineers, and solvent experts everywhere.

Development of the Alternatives Assessment Dashboard.

*Leora Vegosen[1] and **Todd Martin**[2]*
(1)Oak Ridge Institute for Science and Education (ORISE), Oak Ridge, TN, (2)Emerging Chemistry and Engineering Branch, U.S. Environmental Protection Agency, Cincinnati, OH

The goal of alternatives assessment is to identify safer alternatives for chemicals of concern. Comparing chemical hazard profiles (i.e., values for key toxicity categories) is an important component of alternatives assessment. Curating data for a large number of chemicals poses challenges. Several organizations, most notably GreenScreen service providers, perform chemical alternatives assessments and provide user-friendly information for chemical comparison. However, most of these services are not free and are independent of the Environmental Protection Agency (EPA). Therefore, we are developing a user-friendly alternatives assessment tool that merges chemical hazard data from a variety of sources to enable quick comparison of chemicals across several hazard domains.

We obtained chemical hazard data from public online sources and used java programming to parse these data. Chemical hazard data can be in the form of Globally Harmonized System (GHS) scores, the presence of a chemical on one or more lists, quantitative data from one or more toxicity studies, and predicted values based on quantitative structure activity relationships (QSAR). The Toxicity Estimation Software Tool (T.E.S.T.) can provide QSAR estimates for several toxicity endpoints.

Data from multiple sources is used to determine a score (low, medium, high, or very high) for each of several hazard domains (such as acute toxicity, carcinogenicity, etc.). We considered several methods for combining information into one score. The tool enables the scores for different chemicals to be viewed in a succinct color-coded table, providing the capability to quickly compare chemical alternatives. The Alternatives Assessment Dashboard will be implemented in the EPA’s Chemistry Dashboard (https://comptox.epa.gov/dashboard).

Assessing Chemical Alternatives Based on Chemical Structure Using a Name Reaction Database.

***William M. Barrett**[1], Sudhakar Takkellapati[2], Kidus Tadele[2], Leora Vegosen[3], and Michael A. Gonzalez[2]*
(1)U.S. Environmental Protection Agency, Cincinnati, OH, (2)Emerging Chemistry and Engineering Branch, U.S. Environmental Protection Agency, Cincinnati, OH, (3)Oak Ridge Institute for Science and Education (ORISE), Oak Ridge, TN

An alternatives assessment facilitates a comparison of potential alternatives to a chemical of concern. Alternatives assessment should include life-cycle considerations to account for

releases and exposures that occur during the extraction, manufacturing, use, and disposal phases. In the manufacturing phase, processes used to produce a chemical are defined based on the sequence of chemical reactions and unit operations required to form the molecule and separate it from other materials used or produced during its manufacture. Determinations of which reactions are used to form a chemical are made based on the functional groups present in the final molecule. As a result, the releases and exposures from the manufacturing phase of a chemical's life cycle can be evaluated based on the chemical reactions used to form the molecule.

This presentation demonstrates the on-going development and application of a named reaction database to determine the reaction steps required to form a chemical of interest based on the chemical's molecular structure. The reaction steps can then be used to propose the manufacturing process for the chemical, including types and sizes of chemical reactors and separation processes required, feedstock chemicals, by-products, solvents, catalysts, and energy inputs and outputs. Ultimately, the chemical manufacturing processing steps can be tied to a chemical process ontology to estimate releases and exposures occurring during the manufacturing phase of a chemical.

SESSION 7 - PANEL: SUSTAINABILITY BY MANUFACTURING USA INSTITUTES

Wednesday, August 15, 2018
11:30 AM – 12:45 PM
Session Chair: David Shonnard, Michigan Technological University

Sustainability and Process Intensification.

Ignasi Palou-Rivera
RAPID, New York, NY

One can argue that Process Intensification is going through a resurgence. Beyond its European roots and initial development, the establishment of the Rapid Advancement in Process Intensification Deployment (RAPID) Institute (https://www.aiche.org/rapid) by the US Department of Energy represents a critical step. It enables the development of breakthrough technologies to boost energy productivity and energy efficiency through manufacturing processes in industries such oil and gas, pulp and paper and various domestic chemical manufacturers through the use of modular chemical process intensification (MCPI) with the goal of improving productivity and efficiency, cutting operating costs, and reducing waste.

The goals of Process Intensification ("do much more with much less") have many common elements with those of Sustainability and Sustainable Development. It might seem like an obvious conclusion that the use of PI would therefore improve the sustainability characteristics of processes. This talk will explore the thesis of a more complex connection between PI and improvements of sustainability indicators. In fact, some clear tensions between the goals of process intensification and improving the sustainability of the process industries and chemical manufacturing are worth exploring and understanding.

Remanufacturing & the Circular Economy.

Nabil Nasr
REMADE Institute, West Henrietta, NY

Abstract TBA

Sustainability and CESMII.

Haresh Malkani
CESMII, Pittsburgh, PA

The Clean Energy Smart Manufacturing Innovation Institute (CESMII) is one of fourteen Manufacturing USA institutes. Its mission to significantly improve energy consumption in manufacturing through Smart Manufacturing (SM) technologies, business practices and workforce development. The institute has recently approved $16M worth of R&D projects for developing innovative solutions in sensing, control, modeling and analytics applicable across various industry segments. CESMII is also developing a low cost collaborative SM platform that will enable manufacturers, small and large, to rapidly deploy these solutions in their operating facilities. The brief presentation will provide an overview of CESMII, Smart Manufacturing technologies and the SM platform, our current efforts and how the institute helps industrial sustainability.

ICOSSE '18 Poster Presentations

Poster #	Presenting Author(s)	Abstract Title
1	Selorme Agbleze, West Virginia University	*A Computational Framework for Generating Chemical Profile Inventories and Sustainability Assessment in Process Simulators*
2	Catherine B. Almquist and Galen Mahoney, Miami University	*Keratin Protein-Based Adsorbents for the Removal of Heavy Metals from Water*
3	Sharath Ankathi and David Shonnard, Michigan Technological University	*Life Cycle Assessment of Oilseed Crops Produced in Rotation with Dryland Cereals in the Inland Pacific Northwest*
4	Sharath Ankathi and David Shonnard, Michigan Technological University	*Review of Sustainability Impacts for Future Biomethane Production in the US from Anaerobic Digestion of Mixtures of Food Waste and Dairy Manure*
5	Betty Beal and Audrianna Selby, Miami University	*Efforts to Improve the Efficiency of Cookstoves: How Do Additives to Clay Bricks Impact Physical and Thermal Properties?*
6	Shelby Browning, University of Kentucky College of Engineering	*Sustainable Approach for Green Pesticide Production in Kenya from the Croton Megalocarpus Trees*
7	Heriberto Cabezas, Pazmany Peter Catholic University	*Design and Engineering of Sustainable Process Systems and Supply Chains By the P-Graph Framework*
8	Rajat Doshi, Vishwamitra Research Institute	*Application of Adsorbate Solid Solution Theory to Design Novel Adsorbents for Arsenic Removal Using Computer-Aided Molecular Design*
9	Yanhai Du, Kent State University	*Can Fuel Cells Make Our World Cleaner?*
10	Raha Gerami, Wayne State University	*Sustainability Assessment of Automotive Nanocoating Manufacturing: A Case Study on Nanopaint Spray and Curing*
11	Rebecca Hanes, National Renewable Energy Laboratory	*Techno-Economic and Life Cycle Assessment for Guiding Bioenergy Pathway Development*
12	Sage R. Hiibel, University of Nevada Reno	*Water Reuse at Solar Energy Facilities: Impact of Surfactants with Membrane Distillation Treatment*
13	Yicheng Hu, U.S. Environmental Protection Agency, University of Wisconsin-Madison	*Supply Chain Design for Nutrient Management and Harmful Algal Blooms Minimization*
14	Chandni Joshi, University of Kentucky College of Engineering	*Novel Approaches to Waste Plastic Management in Developing Economies*
15	Hannah Margavio, University of Tennessee at Chattanooga	*Determining the Optical and Radiative Properties of Silica Aerogel*
16	Abhijeet Parvatker, Northeastern University	*Building Life-Cycle Inventories for Chemicals with Process Modeling and Statistical Analysis*
17	Evan Pfab, Virginia Commonwealth University	*Microwave Assisted Graphitization of Novel Carbon Support Systems for Cross-Coupling Reactions*
18	Jean Pimentel, Universidad Nacional de Colombia	*P-Graph Approach for Enhancing the Sustainability of Benzaldehyde Production from Toluene Via Reaction-Network Synthesis*
19	John M. Pisciotta, West Chester University	*Electrochemical Nanomaterial Production Coupled to Water Disinfection and Energy Storage*
20	M.Toufiq Reza, Ohio University	*Hydrofew: Hydrothermal Treatment of Wet Wastes into Food-Water-Energy*
21	C. Stewart Slater, Rowan University	*Efficient Production of High Value Added Chemicals and Fuels from Wet Algae*
22	Xin Tan, University of Cincinnati	*Effect of Cell-Free System on Fermentability of Biomass Hydrolysate*
23	Jason Trembly, Ohio University	*Electrochemical Processing to Capture Valuable Nutrients from Animal Feeding Operations Waste*
24	Maobing Tu, University of Cincinnati	*Carbonyl Inhibition of Biofuels Production from Renewable Biomass*
25	Leland Vane, U.S. Environmental Protection Agency	*Membrane-Based Solvent Dehydration to Facilitate Industrial Solvent Reuse and Remanufacturing*
26	Sungwoo Yang, The University of Tennessee at Chattanooga	*Using Radiative Properties of Aerogel to Model Air Water Harvester*
27	Yu Zhang, University of Cincinnati	*Analytical Characterization of Carbonul Inhibitors in Poplar Prehydrolysate By GC-MS*
28	Yu Zhang, University of Cincinnati	*Identification and Quantitation of Carbonyl Inhibitors in Dilute Acid Pretreatment Biomass Hydrolysate Using GC-MS*

ICOSSE ’18 Poster Abstracts

1. A Computational Framework for Generating Chemical Profile Inventories and Sustainability Assessment in Process Simulators.

Selorme Agbleze[1], *Gerardo J. Ruiz-Mercado*[2], *and Fernando V. Lima*[1]
(1)Department of Chemical and Biomedical Engineering, West Virginia University, Morgantown, WV, (2)Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH

Commercial and open-source process simulators have enabled the calculation of mass, energy balances and equipment requirements for chemical process design. These simulators are able to represent steady-state and dynamic processes characterized by high-fidelity models. However, incorporating life cycle inventory information, consisting of release profiles, resource consumption, and production volume, for sustainability assessment and decision-making is currently challenging due to limited capability of process simulators in terms of sustainability features.

In this research, the GREENSCOPE tool Microsoft Excel version, a sustainability assessment tool provided by the U.S. Environmental Protection Agency is enhanced for incorporation into process simulation software to facilitate the generation of life cycle profiles and sustainability assessment of chemical systems. The current GREENSCOPE interface is functional but cumbersome for customers who have limited process systems engineering knowledge. It consists of Excel sheets in which each sheet has multiple cells for user data entries. Integration of the current GREENSCOPE version with process simulation software such as CHEMCAD requires manual exporting of data.

For the improved interface between CHEMCAD and GREENSCOPE, the requirements for each category have been streamlined with similar parameters with dependencies grouped together. Also, built-in values from the GREENSCOPE database are automatically updated on the interface. New plotting capabilities are introduced in which results are shown on plots under their respective categories. In addition, multiple indicators may be combined across categories for plotting. A seamless transfer of data from process simulation software such as CHEMCAD through a Visual Basic for Applications (VBA) link is also implemented based on user definition of input and output streams, to allow for automatic importing of data into GREENSCOPE for observing any LCI and sustainability evaluation changes.

The views expressed in this presentation are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

2. Keratin Protein-Based Adsorbents for the Removal of Heavy Metals from Water.

Catherine B. Almquist[1] *and* ***Galen Mahoney***[2]
(1)Chemical, Paper, Biomedical Engineering, Miami University, Oxford, OH, (2)Miami University, Oxford, OH

Keratin, a natural protein found numerous sources, including skin, hair, nails, hooves, horns, and bird feathers, was investigated as an adsorbent for removing heavy metals from water. The chemical and structural characteristics of keratin allow it to bind with heavy metals. The challenges lie in creating a keratin adsorbent material with high porosity and surface area suitable for water filtration without degrading the adsorption sites on which heavy metals bind.

In this study, we synthesized keratin adsorbents from purchased hair keratin (KeraNetics) and from the keratin extracted from chicken feathers. The keratin was characterized using Scanning Electron Microscopy (SEM) to assess the morphology, Fourier Transform Infrared spectroscopy (FTIR) to assess the functional groups in the keratin structures, thermogravimetric analyses (TGA) to assess thermal stability of the materials, and differential scanning calorimetry (DSC) to assess thermal properties of the materials. Our goal in characterizing the materials was to assess differences in chemical structure of the purchased hair keratin and the keratin extracted from chicken feathers.

We obtained adsorption capacities of the keratin adsorbents as functions of time, temperature, pH, and ionic strength for copper and lead ions in both deionized water and in tap water. In addition, we investigated the competitive adsorption of Cu and Pb on keratin. A thermodynamics assessment was conducted based upon the experimental data and literature. In addition, the relative solubility of the samples was measured.

3. Life Cycle Assessment of Oilseed Crops Produced in Rotation with Dryland Cereals in the Inland Pacific Northwest.

Sharath Ankathi *and* ***David R. Shonnard***
Chemical Engineering, Michigan Technological University, Houghton, MI

Oilseed crops are expected to become an important feedstock for production of renewable jet fuel. The objective of this study is to determine the life cycle energy and greenhouse gas (GHG) emissions of several 2- and 3-year crop rotations with cereals and oilseeds in a low precipitation environment of the inland Pacific Northwest. The purpose is to ascertain whether cropping intensification could improve energy efficiency and reduce GHG emissions.
A life cycle assessment (LCA) was carried out to evaluate the fossil energy and carbon footprint of nine cropping systems. Grain yield and field activity data from cropping systems were acquired from a field experiment over a 5-year period. Inputs for the LCA regarding fertilizers, machinery fuel use, and pesticides were from the field trials and literature for fuel use.

Emission results of winter wheat (WW) rotations are between 300 and 400 g CO2 eq. kg−1 WW, in the range for US average WW cropping emissions (i.e., 300–600 g CO2 eq. kg−1 WW). Reduced tillage fallow (RTF)-Winter oilseed (WO)-RTF-WW and summer fallow (SF)-WW rotation were the most promising, from a trade-off of GHG emissions versus total crop sales over 6 years per hectare with low emissions and high sales. The best oilseed result was 660 g CO2 eq. kg−1 for canola following RTF. Highest yields were observed when cereal or oilseed crops were planted following RTF. Efficiency in terms of Energy Return on Energy Investment was 3.85 for winter oilseed yields 1338.9 kg ha−1 and 1.6 for spring oilseed yields 552.2 kg ha−1
Compared to SF-WW, bioenergy oilseed cultivation may increase CO2 equivalent emissions in 3-year cereal-based rotations due to increased inputs with inclusion of fallow-substitution cultivation. Fossil energy inputs required to produce oilseed crops were smaller than the total energy in final seed and thus oilseeds have the potential to reduce reliance on fossil fuels.

4. Review of Sustainability Impacts for Future Biomethane Production in the US from Anaerobic Digestion of Mixtures of Food Waste and Dairy Manure.

Sharath Ankathi *and* ***David R. Shonnard***
Chemical Engineering, Michigan Technological University, Houghton, MI

Abstract:

Anaerobic Digestion (AD) is a complex set of microbiological and physico-chemical processes to generate biogas, a mixture of predominantly CH_4 (55-65% mol.) and CO_2 (35-45% mol). AD is commercialized globally, however it has limited applications in the U.S. compared to other regions

of the world. AD of mixtures of food waste and animal manure also has great potential to attain economic and environmental benefits compared to other applications of organic waste material processing, such as composting, as shown in a recent environmental life cycle assessment of a commercial biomethane production facility in the state of Colorado in the US (Ankathi et.al, 2017). In that LCA, carbon negative emissions were calculated for biomethane produced from AD of food waste / manure mixtures, with the assumption of avoiding the landfilling of food waste, which is the most likely end of life fate of this material. Specifically, in this paper (and poster) we will discuss the use of AD technology for production of biomethane in different geographic locations, with consideration of socioeconomic and policy factors, technological choices for upgrading biogas to biomethane, and challenges associated with the biomethane supply chain in US (co-location of food waste and dairy manure, proximity to natural gas pipelines for off-take of product, etc.). An in-depth understanding of process modelling and optimization of feedstock blends (Co-digestion) is also provided through this paper as well as feedstock characterization and biogas upgrading technologies. Hence, the objective of this review and poster is to establish a systems perspective on sustainability for biomethane production in the US.

References:

1. Ankathi, Sharath K., James S. Potter, and David R. Shonnard. "Carbon footprint and energy analysis of bio-CH 4 from a mixture of food waste and dairy manure in Denver, Colorado." *Environmental Progress & Sustainable Energy* 37.3 (2018): 1101-1111.

5. Efforts to Improve the Efficiency of Cookstoves: How Do Additives to Clay Bricks Impact Physical and Thermal Properties?.

***Betty Beal**, **Audrianna Selby**, and Catherine B. Almquist*
Chemical, Paper, Biomedical Engineering, Miami University, Oxford, OH

The purpose of the project was to identify a cheap, insulative material for use in a high-efficiency cookstove to reduce the amount of fuel used while still having the stove run efficiently. This was done by investigating the thermal and physical properties of bricks made of clay and clay mixtures. The additives used in the clay mixtures included vermiculite, wood ash, and sawdust. The additives were mixed at two different concentrations to produce six materials of interest for comparison against a baseline material consisting of only clay. Four sample bricks of each material were pre-dried before they were fired in a kiln at 956 C. The bricks were characterized for bulk density, crush compression, water uptake, morphology, and thermal conductivity. The thermal conductivity was measured at steady state using stacked samples between a heat source and a heat sink, with temperature measurements between each layer (heat source, brick, standard material, and heat sink). All temperatures were < 100 C during measurements, and PVC sheet (Type 1) was used as the standard material. The results obtained are supported by the published literature.

6. Sustainable Approach for Green Pesticide Production in Kenya from the Croton Megalocarpus Trees.

***Shelby Browning**[1] and Jeffrey R. Seay, Ph.D., P.E.[2]*
(1)Chemical Engineering, University of Kentucky College of Engineering, Paducah, KY, (2)Chemical and Materials Engineering, University of Kentucky, Paducah, KY

Croton megalocarpus is a nut-producing tree found all over Sub-Saharan Africa. While this tree offers many benefits to the local people such as shade, wind protection, and soil conservation, the inedible nuts it produces have long been thought of as a waste product. Currently, efforts are underway to press oil from the nuts for use as a biofuel, and the left-over seed cake has been found to be a great animal feed product. This still results in a waste product, the husks from the shelled *Croton megalocarpus* nuts. Using a process developed by the University of Kentucky Appropriate Technology and Sustainability (UKATS) research team, those wasted croton nut husks can be converted through slow pyrolysis into a product called wood vinegar. Studies suggest that diluting wood vinegar with water creates an effective non-synthetic pest repellent. The left-over biochar can also be pulverized and added to the soil as an organic fertilizer, resulting in almost a zero-waste use of croton nuts.

The focus of this research is to determine both the effectiveness and the yield of wood vinegar and biochar from *Croton megalocarpus* husks as a function of moisture content, pyrolysis temperature, and the percentage of seeds remaining with the husks after the shelling operation. Response surface methodology (RSM) has been used to construct an experimental plan for the laboratory experiments. The results of this research will be used to analyze the effectiveness of the vinegar as well as optimize the recovery of wood vinegar and biochar from the waste husks.

7. Design and Engineering of Sustainable Process Systems and Supply Chains By the P-Graph Framework.

Heriberto Cabezas[1]*, Andres Argoti*[1]*, Ferenc Friedler*[1]*, Peter Mizsey*[2]*, and Jean Pimentel*[3]
(1)Institute for Process Systems Engineering and Sustainability, Pazmany Peter Catholic University, Budapest, Hungary, (2)Department of Chemical and Environmental Process Engineering, Budapest University of Technology and Economics, Budapest, Hungary, (3)Department of Chemical and Environmental Engineering, Universidad Nacional de Colombia, Bogota, Colombia

The design of sustainable manufacturing processes and supply chains is rapidly becoming a critical issue. The reason is the necessity of providing for the needs of a growing human population which is increasingly prosperous across the globe. To this purpose, this review article explores the most important elements of sustainability science and couples them with the P-graph framework, thereby rendering it possible to design feasible process and supply structures with great ease. Structure is an often-overlooked aspect of process and supply chain design, in part because even relative simple processes or supply chains can have an enormous number of feasible structures. We further illustrate the application of these ideas with examples of energy generation processes and supply chains.[1]

[1] Cabezas, H., Argoti, A., Friedler, F., Mizsey, P, and J.P. Pimentel, "Design and Engineering of Sustainable Process Systems and Supply Chains by the P-Graph Framework," Env. Prog. Sust. Energy, in press. DOI: 10.1002/ep.12763.

8. Application of Adsorbate Solid Solution Theory to Design Novel Adsorbents for Arsenic Removal Using Computer-Aided Molecular Design.

Rajat Doshi[1]*, Rajib Mukherjee*[2]*, Urmila M. Diwekar*[3]*, Suresh Gupta*[4]*, and Arti A. Rajput*[5]
(1)Vishwamitra Research Institute, Tampa, FL, (2)VRI-CUSTOM, Crystal Lake, IL, (3)Vishwamitra Research Institute, Clarendon Hills, IL, (4)Chemical Engineering, Birla Institute of Technology & Science, Pilani, Pilani, India, (5)Chemical Engineering, BITS Pilani, Pilani, India

Arsenic is a carcinogenic contaminant that pollutes the groundwater, a consequence of poor arsenic disposal. Current arsenic separating agents have a limited adsorption capacity. The overall objective of this work is to develop a computational tool for the design of novel adsorbents for arsenic remediation using clay materials including beidellite, zeolite, and sepiolite that are cheap and readily available. In the first part of this research, we use the Group Contribution Method (GCM) to predict thermodynamic properties and calculate the UNIFAC interaction parameters between arsenic and selected functional groups. In the second part of this research, we utilize a computer-aided molecular design (CAMD) that develops new adsorbent candidates with enhanced adsorption capacities based on UNIFAC interaction parameters generated in the first part. The efficient ant colony optimization (EACO) algorithm maximizes the adsorption capacity with certain structural possibilities, thermodynamic constraints, and process conditions. It was found that the newly designed adsorbent has an order of magnitude higher removal capacity than the adsorbents' reported in the literature. The adsorption capacity estimated for the designed adsorbent was simulated in groundwater conditions; however, arsenic contamination is not solely confined to groundwater since it is also highly prevalent in wastewater flows from coal-burning plants. An expansion of our work will be carried out by conducting experiments on the designed adsorbents. The goal is to test the performance of the designed adsorbent in coal-burning plant's wastewater flows to understand how the different ionic environment affects the adsorption capacity. Moreover, the novel adsorbent has also been synthetically prototyped to determine the actual adsorption capacity of the novel adsorbent in varying ionic environments and arsenic concentrations. Our initial results from experimentation has demonstrated an enhanced adsorption capacity of the synthetic adsorbent that exceeds that of any naturally occurring adsorbent.

9. Can Fuel Cells Make Our World Cleaner?

Yanhai Du
Applied Engineering, Kent State University, Kent, OH

Today our world runs mainly on fossil fuels which release greenhouse gases and cause global warming. Majority of electricity comes from burning coal and/or natural gas. This picture may not change in the decades to come even the renewables increase in a very fast pace. Fuel cell technology is seen as one of the most efficient way to convert chemical energy in fossil fuels into electricity. This is because the energy conversion through a fuel cell is direct and without combustion. In comparing with the conventional thermal process, fuel cells could be two to three times as efficient as burning the fuels.

This presentation will show how fuel cells can fit perfectly to our fossil fuel energy era and bring an excellent solution to maintain our economy growing needs of energy while dramatically cut down the greenhouse emissions, and contribute to a greener and more sustainable world.

10. Techno-Economic and Life Cycle Assessment for Guiding Bioenergy Pathway Development.

***Rebecca Hanes**[1], Nicholas Grundl[2], and Mary Biddy[2]*
(1)Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO, (2)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO

The Center for Bioenergy Innovation (CBI) is a bioenergy research center recently launched by the U.S. Department of Energy Office of Science's Biological and Environmental Research program. CBI's objective is to enable innovations across the bioenergy supply chain through development of poplar and switchgrass phenotypes, microorganisms for consolidated bio-processing (CBP), in which biomass fermentation and conversion is accomplished in a single unit operation, and lignin valorization processes. In addition to basic science, CBI's activities involve the application of techno-economic analysis (TEA) and life cycle assessment (LCA) to the bioenergy pathways under study. TEA and LCA is used to quantify the impacts that research and development breakthroughs have on the economic

viability and sustainability of a bioenergy pathway, and to identify drivers for reducing costs and improving sustainability through targeted research efforts. Combining TEA and LCA allows for understanding the economic and sustainability benefits and trade-offs of these integrated bioenergy systems.

The focus of this presentation is a parameterized, integrated TEA-LCA model, which will be discussed along with an application to bioenergy pathways currently under study. The model combines data and information developed by CBI researchers into a superstructure of potential bioenergy pathways and their life cycles. Model parameters include feedstock species and phenotype, farming, harvesting, storage and transportation practices, and the microbes used for biomass conversion and lignin valorization, among others. The parameterized TEA-LCA model allows for the rapid quantification of pathway economic and sustainability metrics such as minimum fuel selling price, payback period, fossil fuel consumption and net greenhouse gas emissions. To demonstrate the model, economic and sustainability metrics for a bioenergy pathway utilizing CBP will be quantified and compared to the same metrics for a conventional bioenergy pathway. Results of the comparison will be used to identify and prioritize high-impact research areas within the CBP pathway.

11. Sustainability Assessment of Automotive Nanocoating Manufacturing: A Case Study on Nanopaint Spray and Curing.

***Raha Gerami*[1], *Illya Salinnyk*[2] *and Yinlun Huang*[1]
(1) Department of Chemical Engineering and Materials Science, Wayne State University, Detroit, MI (2) Florida Institute of Technology, Melbourne, Florida

Nanopaint is a new, attractive coating material in the automotive coating industry, as when it is applied on vehicle surface, the resulting nanocoating layer(s), through a number of manufacturing steps, could possess a number of enhanced or even new properties and functional capacities. However, there could exist a number of serious environmental concerns, as during the nanopaint manufacturing and application phases, nanoparticles in paint and coating layers could enter the working environment through emission into air and water. A further concern is the nanoparticle release into the environment during the product use phase. The unintended environmental and health risks, as well as the economic and social challenges associated with the use of nanocoating products, should be systematically estimated.

In this paper, we present our recent progress on nanocoating sustainability by focusing on the nanocoating manufacturing process and product performance. We propose a sustainability metrics system that could be used to provide a more comprehensive assessment of the environmental, economic, and social performances of the manufacturing process and the product. We will also introduce a framework of multiscale sustainability analysis nanocoating manufacturing and application, where individual manufacturing objectives are allocated at the appropriate scales of length and time. The correlations among paint material, paint spray, coating curing, and product performance are identified. A comprehensive case study on nanopaint spray and curing will be presented to show methodological efficacy.

12. Water Reuse at Solar Energy Facilities: Impact of Surfactants with Membrane Distillation Treatment.

Coral R. Taylor[1], *Pejman Ahmadiannamini*[2], *and* ***Sage R. Hiibel***[3]
(1)Civil and Environmental Engineering, University of Nevada, Reno, Reno, NV, (2)Chemical and Materials Engineering, University of Nevada, Reno, Reno, NV, (3)Civil and Environmental Engineering, University of Nevada Reno, Reno, NV

Solar energy facilities (SEF) utilize water for cooling and cleaning of panels and mirrors to improve solar efficiency, however water resources and treatment infrastructure are typically lacking in areas where SEFs are located. For panel cleaning, high-quality water is necessary as particles or dissolved salts can leave residuals on the panels, counteracting the benefits of cleaning. Thus, an on-site treatment method that provides a high-quality water while removing heat from the panels is needed.

Membrane distillation (MD) is a potential SEF water treatment option that uses a hydrophobic, microporous membrane to separate a warm, dirty feed water from a cool, clean distillate water; the temperature difference across the membrane leads to a vapor pressure difference that drives transport of water vapor through the membrane while rejecting molecules less volatile than water. At SEFs, the 'dirty' water can be used for panel cooling, which serves as a pre-heating mechanism for MD, and the high-quality distillate water from MD can be used for panel washing. However, as part of the panel wash, surfactants are often used to improve cleaning efficiencies, and due to limited water resources at many SEFs, the panel wash water is captured for on-site reuse. The resulting low-levels of surfactants are a challenge for MD, as surfactants accumulate at the membrane surface and decrease hydrophobicity, which ultimately can result in pore wetting and decreased membrane performance.

The effects of anionic and non-surfactants on range of membranes of various materials and pore sizes were evaluated. The surfactant concentration at which the onset of pore wetting occurred was determined using a novel graphical method, and verified spectrophotometrically. Overall, the membrane material and surfactant type had the biggest impact on MD performance. PTFE membranes generally tolerated higher surfactant concentrations, and all membranes were more sensitive to anionic surfactants than to non-ionic surfactants.

13. Supply Chain Design for Nutrient Management and Harmful Algal Blooms Minimization.

Yicheng Hu[1,2]*, Apoorva Sampat*[2]*, Victor M. Zavala*[2]*, and Gerardo J. Ruiz-Mercado*[3]
(1)National Risk Management Research Laboratory, U.S. Environmental Protection Agency, Cincinnati, OH, (2)Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI, (3)Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH

The harmful algal blooms (HABs) is a universal and complex problem throughout the world. The HABs can lead to severe human health threats and enormous remediation costs by generating toxicity risk for humans, aquatic life, decreasing economic value of recreational water systems due to color, and odor issues. It is estimated that 30% of lakes from 36 states in the US have reported HABs problems and the corresponding tourism losses and commercial fishing losses reached one billion and more than ten million dollars per year respectively.

In this project, we combine multiple types of modeling tools to analyze the relationship between nutrient management strategies from organic waste and HABs. The first part is a supply chain modeling framework, which captures the balance and transformation of waste, nutrient, and product at each location, waste transportation, and technology selection and placement. This supply chain model can achieve the coordination among stakeholders with different objectives by minimizing a weighted summation of direct economic costs, health threats, and environmental impacts caused by HABs. The second part is a nutrient transport model, which can track the fate and transport process of nutrients from the soil to aquatic systems. The third part is an algal bloom prediction model to relate the nutrient concentration and other natural factors (temperature, sunlight, etc.) and algal bloom level.

Finally, we compared the predicted algal bloom level with threshold suggested by US EPA to analyze the HABs response to nutrient management actions. We will present a series of real case studies in the Yahara Watershed in the State of Wisconsin to illustrate the model structure and practicability.

14. Novel Approaches to Waste Plastic Management in Developing Economies.

Chandni Joshi[1] *and Jeffrey R. Seay, Ph.D., P.E.*[2]
(1)Chemical Engineering, University of Kentucky College of Engineering, Paducah, KY, (2)Chemical and Materials Engineering, University of Kentucky, Paducah, KY

Municipal solid waste accumulation is a major challenge for governmental municipalities of developing countries, where population growth, urbanization, capital and infrastructure constraints, poor regulation and waste management education challenge the way waste is collected, recycled and disposed. Plastic accumulation further poses a threat due to limited land availability for landfilling, leading to serious health and environmental consequences when dumped on open plots of land/streets. This research applies a Trash to Tank approach for plastic waste management in developing economies. Trash to Tank is a concept based on the conversion of waste plastic into a liquid fuel via appropriate technology, suitable as an alternative for diesel or kerosene fuel applications. This research presents a case study on the use of this approach in Kampala, Uganda to analyze the feasibility, challenges and benefits associated with implementation in both urban and rural regions. The differences amongst these regions is compared, along with an assessment of fuel combustion emissions, entrepreneurial advantages and social acceptance.

15. Determining the Optical and Radiative Properties of Silica Aerogel.

Hannah Margavio
Civil & Chemical Engineering, University of Tennessee at Chattanooga, Chattanooga, TN

Silica aerogel is a highly porous, optically transparent, low density, thermally insulating rubber-like polymer material. These properties make the material an excellent candidate for an energy-efficient window when bonded to glass, because if less thermal radiation is transmitted to the interior from the outside, then less energy is required to heat or cool the room. Before building a prototype of the window, it is important to decouple the extinction of a beam of incident radiation, since only scattering of radiation is considered in many models. In my model, extinction of the incident light beam is due to scattering and absorption of light due to the aerogel's high density of inter-crystalline pores, which effectively "trap" radiation. To solve this, I have written a program in Python which solves the radiative transfer equation for the total field of intensity of radiation by 10-point Guassian Quadrature integration, and using input of albedo and optical thickness, the program will output the transmissivity and reflectivity of the silica aerogel at several different optical thicknesses. Doing this will help me and my team determine the optimal thickness of silica aerogel to use for a window to yield the desired transmissivity.

16. Building Life-Cycle Inventories for Chemicals with Process Modeling and Statistical Analysis.

Abhijeet Parvatker[1] *and Matthew J. Eckelman*[2]
(1)Chemical Engineering, Northeastern University, Boston, MA, (2)Civil & Environmental Engineering, Northeastern University, Boston, MA

Developing rapid but robust life cycle inventory (LCI) data for chemicals in the absence of primary data from manufacturing has been a major challenge for life cycle assessment (LCA) practitioners. The limited data available in LCI databases cover less than 1% of the chemicals manufactured and traded in the market today. While basic calculations based on reaction stoichiometry fail to account for the process energy requirements, more sophisticated approaches such as process simulation are time consuming and restricted by the availability of required parameters. Other rapid approaches such as molecular structure-based models are empirical rather than mechanistic and tend to provide results in terms of limited impact categories rather than full LCI data. In this work, we combine synthesis trees, process calculations, and multi-variate statistical methods in order to develop an LCI data generation tool for organic chemicals. LCI data categories include reactants, other chemical inputs such as solvents, process heat required, and electrical energy used. Statistical models were built using primary data from industrial chemistry texts, supported by simulations for more than 50 different chemical reactions using AspenPlus to determine the energy requirements. Multiple regression analysis was used to determine the coefficients of energy use based on key reaction parameters such heat of reaction, specific heat of the reactants and temperature of the reaction. High correlation was found between heat of reaction and reaction energy, with R^2 in the range of 0.8-0.9 for most processes studied. The prediction accuracy with other parameter, which are considered more likely to influence the energy use, such as specific heat and temperature, were relatively low with R^2 in the range of 0.3-0.5. Analysis in this work provide key insights into the gate-to-gate energy calculations for chemical processes which is one of the critical inputs in a chemical LCI.

17. Microwave Assisted Graphitization of Novel Carbon Support Systems for Cross-Coupling Reactions.

Evan Pfab*, Sarah Smith, Stanley Gilliland III, and Frank Gupton*
Chemical and Life Science Engineering, Virginia Commonwealth University, Richmond, VA

Palladium catalysts are widely used in industry to facilitate many necessary reactions. With recent pushes towards better efficiency and improved sustainability, heterogeneous palladium catalysts have been of particular focus. A crucial component of this development has been identifying effective solid support systems. Graphene is an excellent solid support that has also shown to enhance catalytic activity, but the high cost makes it less practical. A promising approach to this issue is the graphitization of lower grade carbons. After dispersing Pd onto carbon black via strong electrostatic adsorption, we have used microwave irradiation treatments to demonstrate graphitization. These graphitized carbon supports offer improved catalytic activity in Pd-catalyzed cross-coupling reactions.

18. P-Graph Approach for Enhancing the Sustainability of Benzaldehyde Production from Toluene Via Reaction-Network Synthesis.

Jean Pimentel*[1], Andres Argoti[2], Ivan Gil[1], Istvan Heckl[3], Botond Bertok[3], Ferenc Friedler[2], and Juan Carlos Garcia-Ojeda[4]*
(1)Department of Chemical and Environmental Engineering, Grupo de Procesos Químicos y Bioquímicos, Universidad Nacional de Colombia, Bogotá, Colombia, (2)Institute for Process Systems Engineering and Sustainability, Pazmany Peter Catholic University, Budapest, Hungary, (3)Department of Computer Science and Systems Technology, University of Pannonia, Veszprem, Hungary, (4)Facultad de Ingeniería de Telecomunicaciones, Universidad Santo Tomás, Bucaramanga, Colombia

Herein, we aim at synthesizing the optimal and near-optimal reaction networks to manufacture benzaldehyde from toluene from a set of reactions of industrial interest. In this regard, we expect that the reaction networks optimally synthesized will significantly reduce the consumption of hazardous materials, thereby increasing the process' sustainability. To synthesize such reaction networks, we adapt the methodology for process-network synthesis (PNS) in light of the P-graph framework; this adaptation is referred to as reaction-network synthesis (RNS) accordingly. At the outset of RNS, the feasible reaction networks are selected from the set of all plausible reactions of industrial significance producing benzaldehyde from toluene available in the literature. Moreover, the reactions selected are stoichiometrically balanced and depicted as P-graphs, thereby graphically representing the reacting species, i.e., reactants and products. Subsequently, the superstructure formed by combining the P-graphs of the feasible reactions is generated by executing algorithm maximal-structure generation (MSG). In addition, the combinatorially and stoichiometrically feasible reaction networks are determined from the superstructure with algorithm solution-structure generation (SSG) and integer linear programming (LP). Finally, the optimal and near-optimal reaction networks are identified from those stoichiometrically feasible with an objective function defined in terms of the profit that could be obtained from the reactions. In this regard, the objective function embeds the reaction networks' environmental impact and safety by means of suitable metrics, such as the global-warming potential, explosiveness factor, and aquatic-toxicity potential.

19. Electrochemical Nanomaterial Production Coupled to Water Disinfection and Energy Storage.

John M. Pisciotta
Biology, West Chester University, West Chester, PA

Access to clean water is a human right threatened by increasing fossil fuel based industrialization and lack of adequate water treatment and sanitation in many areas. Here we investigate a renewable energy storage method designed to disinfect water while electrochemically upcycling scrap metal into useful nanomaterial. The aim is coupling renewable energy storage and metal nanoparticle synthesis for use at the food, energy, water nexus. Glass vials were filled with 80 mL of 100 mM NaCl and fitted with a 5-cm piece of copper (Cathode) and a 7.5 cm piece of iron (Anode). Electrodes were sterilized by alcohol and were punctured through rubber stoppers. Vials were attached to a power supply and individual vials exposed to voltages of 0V, 5V, 10V or 15V for 10 minutes. GC analysis revealed 108 ml/hr H2 production at 15 volts. Concurrent with H2 production, a green precipitate formed. X ray diffraction analysis of the dried precipitate revealed it to be primarily crystalline Cu2(OH)3Cl. SEM further indicated crystalline, amorphous structures consistent with Cu2(OH)3Cl, also known as tribasic copper chloride (TBCC), the mineral atacamite. Bacteria spiked into this aqueous system were inactivated. This study demonstrates the technical effectiveness of the system as a method to store energy as H2 while disinfecting water and forming a useful product. TBCC is a metal based anti-microbial widely used today for crop protection as a fungicide. Waste scrap metal is widespread and the collection and upcycling of waste metals to operate energy storage and water treatment devices of the design proposed here provides an incentive to clean up landscapes and reduce hazards. Production of TBCC was achieved with coupled water disinfection and attendant H2 based energy storage.

20. Hydrofew: Hydrothermal Treatment of Wet Wastes into Food-Water-Energy.

***M.Toufiq Reza**[1], Kyle McGaughy[2], Pretom Saha[1], Akbar Saba[1], and Nepu Saha[3]*
(1)Mechanical Engineering, Ohio University, Athens, OH, (2)Chemical and Biomedical Engineering, Ohio University, Athens, OH, (3)Chemical Engineering, Ohio University, Athens, OH

The world has been producing nearly 2 billion tons of garbage also known as municipal solid waste (MSW) per year. Garbage contains mainly non-recyclable organic fraction (OFMSW) and the

composition can add up to 70 % of MSW. Except from some cases, where OFMSW has been composted or anaerobically digested, it ends up in landfills, where it contributes to environmental pollution via greenhouse gases (mainly methane and carbon dioxide). Although OFMSW has huge potential for food-energy-water (FEW) production, converting it to FEW in both efficiently and economically manner remains a challenge.

Hydrothermal carbonization (HTC) is an exceptional treatment process for biofuel production, as residual water is the reaction media for HTC. Therefore, the wet biomass need not be dried prior to the HTC. Subcritical water at around 200-260 °C has the highest ionic constant, which means it is quite reactive. As a result, within 5 minutes of reaction with biomass, solid product is formed along with HTC process liquid and gaseous byproducts. Over the past year, hydrochar has been gasified to produce synthesis gas by our group. We will present the gasification kinetics and gas composition in this presentation. Furthermore, we are also studying deep eutectic solvents (DES) for carbon dioxide capture from gas streams such as syn-gas. One of the major benefits of DES is the lower capital and regeneration cost. This will allow us to purify syngas and carbon dioxide for further applications. HTC process liquid has been proven effective on freshwater algae growth. *Chlorella sp.* has been cultivated in HTC process liquid. The resulted water has very low COD and nutrient loading. Our future goals are to produce irrigation quality water from HTC process liquid and to produce algae for animal feeding.

21. Efficient Production of High Value Added Chemicals and Fuels from Wet Algae.

***C. Stewart Slater*[1]**, *Harrison Hawkins[2], Alexander Johnson[2], Amanda Christon[2], Kauser Jahan[3], Mariano Savelski[2], and Iman Noshadi[2]*
(1)Department of Chemical Engineering, Rowan University, Glassboro, NJ, (2)Chemical Engineering, Rowan University, Glassboro, NJ, (3)Civil and Environmental Engineering, Rowan University, Glassboro, NJ

Short chain diols like ethylene glycol, propanediol (PDO), butanediols (BDO), are of great importance as platform chemicals for intermediates, polymers and building block chemicals. The shift towards reduced fossil fuel dependence is expected to enhance bio-renewable chemical market growth. Global 1,3 PDO market is estimated to register a CAGR of 10.4% between 2014 and 2021 while its market escalates to $760 million by 2022. Bioprocesses to produce short-chain diols from renewable carbon sources are attracting interest as a topic of current research. A case in point is Dupont's glucose fermentation to 1,3-PDO by genetically modified bacteria E. Coli. Bacteria of Lactobacillus, Clostridium, and Citobacter genus produce 1,3 PDO and hydrogen from glycerol, sugars or feeds containing both. A major process challenge lies in enriching fermentation products from dilute aqueous mixtures. Conventional separation techniques have higher cost and energy consumption and hence applicability. Membrane separation processes are inexpensive and energy efficient in enriching components from dilute mixtures. Pervaporation is energetically advantageous, but all fermentation products cannot be enriched by conventional membrane materials. Novel polymer development is essential to establish sustainable industrial separation procedures. We developed an integrated extraction – fermentation – separation process for deriving carbohydrates from biomass, their conversion to diols and subsequent purification and enrichment of the fermentation products by membrane pervaporation, with process optimization for maximum productivity and yield. This report outlines the synthesis of a novel hydrophobic imidazolium dibutylphosphate ionic liquid based acrylate monomer for the pervaporative enrichment of 1,3-propanediol (1,3-PD) from dilute aqueous mixtures. This monomer provides an inexpensive alternative to current high performing pervaporative materials. Based on its high 1,3-PD affinity, hydrophobic nature, and excellent cost, this polymer is an attractive candidate for a variety of industrial applications.

22. Effect of Cell-Free System on Fermentability of Biomass Hydrolysate.

Xin Tan[1] *and Maobing Tu*[2]
(1)Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH, (2)Center for Bioenergy and Bioproducts, Auburn University, Auburn, AL

A broad range of inhibitory compounds released in the biomass pretreatment significantly inhibit the production rate of ethanol in yeast fermentation. In order to overcome the effect of inhibitors, many strategies that include improvement of natural tolerance of yeast have been developed. Cell-free system was reported to be more controllable and have higher environmental tolerance than intact cell in alcoholic fermentation. In this study, the effect of yeast cell-free system on hemicellulose hydrolysates fermentation was studied. Impressively, the cell-free system enhanced bio-ethanol production in hemicellulose hydrolysate. It was observed that cell-free yeast extracts consumed all the glucose in the undetoxifed hydrolysates within 12 h and produced 9.5 g/l of ethanol, but the intact yeast could not ferment the undetoxifed hydrolysates. The potential mechanism of this promotion in ethanol production may be that the cell free system could eliminate the inhibitory effect of hydrolysate on yeast glucose transport. It was noticed that the glucose transport was completely stopped in the hemicellulose hydrolysate. No intracellular glucose was detected in yeast after incubation with the undetoxifed hydrolysates, while 46 mg/g intracellular glucose was presented inside of yeast after incubation with the detoxified hydrolysates. This study indicated that the cell free system has higher bioethanol productivity because it could avoid the inhibition of toxic compounds on the glucose transport step.

23. Electrochemical Processing to Capture Valuable Nutrients from Animal Feeding Operations Waste.

Jason Trembly *and Zineb Belarbi*
Institute for Sustainable Energy and the Environment, Ohio University, Athens, OH

Land application of manure is a beneficial practice which improves soil quality by recycling important nutrients found in animal waste. Eutrophication of water resources caused by nutrient runoff, mainly phosphorus (P) and nitrogen (N), from soil conditioned with animal manure is a growing national problem. Recovering a portion of the manure's nutrient content before land application could help alleviate both nutrient runoff pollution and concentrated animal feeding operations (CAFO) permitting limitations.

Nutrient recovery technologies must be able to easily integrate within existing CAFO infrastructure, possess low capital/operating costs, not interfere with operation, and generate a reusable nutrient product which can be directly applied to land. Electrochemical-based processes offer several advantages including compact/modular design, selective removal, and simple operation. The overall objective of the present research is to evaluate the ability to utilize an electrochemical-based approach to selectively recover P and N from animal waste as a solid struvite ($MgNH_4PO_4 \cdot 6H_2O$) fertilizer product.

This presentation will present results utilizing lab-scale electrochemical reactors to evaluate the effectiveness of recovering struvite from animal waste. The effect of applied potential, turbulent flow, waste composition, and temperature on the kinetics of struvite precipitation will be presented. Further, power requirements associated with nutrient recovery and preliminary process economics will be discussed. Results indicate this approach could offer CAFOs a modular technology which smoothly integrates into current manure lagoon systems. Key parameters controlling electrochemical struvite precipitation include: solution pH, temperature, turbulence, and the presence of competing ions (Ca^{2+}).

24. Carbonyl Inhibition of Biofuels Production from Renewable Biomass.

Maobing Tu
Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH

Developing biofuels from renewable biomass has great potential to reduce U.S. dependence on fossil oil while improving national energy security and addressing the environmental issues. The Renewable Fuel Standard mandates 36 billion gallons of biofuels should be produced annually by 2022, with 16 billion gallons coming from lignocellulosic biomass. Ethanol and butanol are the promising advanced biofuels being pursued by the DOE, NSF and USDA for the next generation of alternative fuels. However, one of the major bottlenecks impeding production of viable biofuels from renewable biomass is the lack of cost-effective processes for converting biomass into biofuels.

Biomass pretreatment is needed to break down the recalcitrant structure of the plant cell wall for subsequent enzymatic hydrolysis and fermentation. However, the pretreatment processes generate inhibitors from the degradation of cellulose, hemicellulose, lignin and extractives, many of which significantly reduce the microbial growth and fermentation productivity during the fermentation process. Detoxification or conditioning methods are required to reduce the toxicity of hydrolysates for biofuels fermentation, but they increase the total production cost significantly. Progress has been made in the identification of hydrolysates inhibitors. However, the compounds identified to date cannot account for the inhibition level in real biomass hydrolysates and the most potent inhibitors remain elusive. Equally important, little is known about the reaction mechanisms of overliming and ammonia detoxification for biomass hydrolysates despite both methods being widely used in biofuels and chemical production. Therefore, there is a critical need to better understand the chemistry of biomass-derived inhibitors in the bioconversion processes. Although most identified inhibitors belong to carbonyl compounds, surprisingly the classification of inhibitors has not been correlated to carbonyls. The structure and functional groups in carbonyls will most likely govern the reactivity of carbonyl compounds, and the reactivity of carbonyls will potentially dominate their inhibitory effects on microbial fermentation.

25. Membrane-Based Solvent Dehydration to Facilitate Industrial Solvent Reuse and Remanufacturing.

Leland Vane[1]*, Franklin Alvarez*[1]*, Vasudevan V. Namboodiri*[1]*, and Michael Abar*[2]
(1)National Risk Management Research Laboratory, U.S. Environmental Protection Agency, Cincinnati, OH, (2)NCOA, Cincinnati, OH

Organic solvents serve a variety of functions in the manufacture of materials and products. The life cycle of industrial solvents presents sources of emissions that potentially impact human health and the environment. If solvent use cannot be avoided, the Green Chemistry/Engineering principles advocate employing the least amount of the safest solvent that delivers the requisite performance. In many situations, the life cycle impact of using even the safest solvents can be reduced further by recovering and reusing the solvents.

The Remanufacturing Exclusion of the EPA's *New Definition of Solid Waste* rule is intended, in part, to promote the reuse/reprocessing of 18 solvents in the pharmaceutical, paint/coating, plastic/resin, and basic organic chemical sectors(1). The technical challenge is that replacing virgin solvents with reclaimed material requires separation technologies to recover those solvents from their mixtures with other processing materials, such as water, and to purify them to meet reuse specifications. These separation technologies present an environmental opportunity but also an environmental challenge because they each have an environmental footprint, the largest footprint often due to energy usage.

Research at the EPA's National Risk Management Research Laboratory on the review, development, and evaluation of advanced separation materials/technologies for energy-efficient solvent reprocessing will be described. Solvent/water mixtures will be emphasized because most of the solvents identified in the definition of Solid Waste rule form difficult-to-separate azeotropic mixtures with water. The research is an extension of successful in-house development of membrane-based processes and materials to efficiently recover and dry alcohol-based biofuels, several of which are among the 18 industrial solvents targeted here.

(1) https://www.epa.gov/hwgenerators/final-rule-2015-definition-solid-waste-dsw

The views expressed in this abstract are those of the authors and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency.

26. Using Radiative Properties of Aerogel to Model Air Water Harvester.

Sungwoo Yang
Civil & Chemical Engineering, The University of Tennessee at Chattanooga, Chattanooga, TN

Silica aerogel is a highly porous, low density material which absorbs light and scatters it in all directions of propagation. It is also optically transparent and thermally insulating due to these intrinsic properties of the molecular structure. This makes silica aerogel an excellent material to bond to windows to make glass structures more energy efficient by lowering heating and cooling costs. Before modelling transmittance and reflectance, we must understand that because of the high porosity of silica aerogel, we witness the multiple scattering effect, so to model the optical properties, we must model hemispherical transmittance and reflectance as the sum of forward and backward scattering intensities of the incident light beam through the material. To obtain the total intensity field, we call upon the radiative transfer equation (RTE) which states that the cosine of the polar angle with respect to the incident direction times the partial derivative of wavelength dependent intensity with respect to optical depth is equal to the negative intensity field over the optical depth and cosines of the polar angles to the incident directions plus one half albedo times the integral of the intensity field from negative one to one. We can solve the integro-differential equation for the intensity field by Gaussian-Legendre Quadrature, a method of numerical integration. I have written a program in python which computes the intensity field using the method of numerical integration, and then solving for hemispherical transmittance and reflectance. After plotting transmittance with albedo and optical depth and reflectance with albedo and optical depth, we super impose the images to see the curves intersect at one point, giving an albedo and optical depth we can use to model the coefficients of scattering and absorption.

27. Analytical Characterization of Carbonul Inhibitors in Poplar Prehydrolysate By GC-MS.

***Yu Zhang**, Maobing Tu, and Changlei Xia*
Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH

A variety amount of degradation compounds was generated upon the biomass pretreatment process. The carbonyl compounds (aldehydes and ketones)

have been suggested to the major inhibitors because of their significantly inhibitory influence on the microbial fermentation. However, the identification of the most potent carbonyl inhibitors has been challenged because of their low concentrations and difficult separation from biomass hydrolysates. In this study, we developed an analytical method that enabled the identification and quantitation of more than 50 carbonyl inhibitors (including furans, aliphatic derivatives, aromatic monomers and aromatic dimers) in dilute acid pretreated poplar hydrolysate by gas chromatography-mass spectrometry (GC-MS). The carbonyl inhibitors were extracted by dimethyl chloride (DCM) and concentrated by nitrogen blowing. However, the low concertation of some carbonyl inhibitors impeded their identification since their signals might be obscured by other compounds. Herein, a reactive extraction using saturated $NaHSO_3$ has been developed to selectively separate aldehydes/ketones from biomass hydrolysates through a revisable reaction. The reacted bisulfite adducts were precipitated and hydrolysed back to aldehydes/ketones by HCl. The separated aldehydes/ketones were further extracted by DCM and analysed by GC-MS. The separation of aldehyde/ketone compounds offered more flexibility and potential to condense the low-concertation but high reactivity aldehydes/ketones for easier identification (e.g. 2,3-dihydroxybenzaldehyde and 2'-hydroxy- 6'-methoxyacetophenone). The identification and quantitation approach in this study greatly favor the understanding of the inhibition of the biomass hydrolysate, as well as the effect of detoxification methods on microbial fermentation.

28. Identification and Quantitation of Carbonyl Inhibitors in Dilute Acid Pretreatment Biomass Hydrolysate Using GC-MS.

Yu Zhang*, Maobing Tu, and Changlei Xia*
Chemical and Environmental Engineering, University of Cincinnati, Cincinnati, OH

A variety amount of degradation compounds was generated upon the biomass pretreatment process. The carbonyl compounds (aldehydes and ketones) have been suggested to the major inhibitors because of their significantly inhibitory influence on the microbial fermentation. However, the identification of the most potent carbonyl inhibitors has been challenged because of their low concentrations and difficult separation from biomass hydrolysates. In this study, we developed an analytical method that enabled the identification and quantitation of more than 50 carbonyl inhibitors (including furans, aliphatic derivatives, aromatic monomers and aromatic dimers) in dilute acid pretreated poplar hydrolysate by gas chromatography-mass spectrometry (GC-MS). The carbonyl inhibitors were extracted by dimethyl chloride (DCM) and concentrated by nitrogen blowing. However, the low concertation of some carbonyl inhibitors impeded their identification since their signals might be obscured by other compounds. Herein, a reactive extraction using saturated $NaHSO_3$ has been developed to selectively separate aldehydes/ketones from biomass hydrolysates through a revisable reaction. The reacted bisulfite adducts were precipitated and hydrolysed back to aldehydes/ketones by HCl. The separated aldehydes/ketones were further extracted by DCM and analysed by GC-MS. The separation of aldehyde/ketone compounds offered more flexibility and potential to condense the low-concertation but high reactivity aldehydes/ketones for easier identification (e.g. 2,3-dihydroxybenzaldehyde and 2'-hydroxy- 6'-methoxyacetophenone). The identification and quantitation approach in this study greatly favor the understanding of the inhibition of the biomass hydrolysate, as well as the effect of detoxification methods on microbial fermentation.

ICOSSE '18 Speaker Biographies

Plenary Speakers

Oliver Kroner, Green Cincinnati Plan & Sustainability Coordinator, City of Cincinnati

Oliver Kroner is the Sustainability Coordinator for the City of Cincinnati, where he works with city government and community members to identify and implement strategies to prepare the City for the future. He is responsible for advancing and tracking the sustainability and resiliency recommendations of the Green Cincinnati Plan, including greenhouse gas modeling. Prior to this role, he worked as an Environmental Scientist with the University of Cincinnati's Risk Science Center, modeling the human health impacts of chemicals in the environment. He serves on the boards of the Green Partnership for Greater Cincinnati, and the Mill Creek Alliance. Previous board roles have included Northside Community Council (President), Fuel Cincinnati, and PAR Projects. He is a graduate of Miami University and Northeastern University, and a proud AmeriCorps alum.

Tracy Young, Global R&D Director, Construction Chemicals & Cellulosics Technology, The Dow Chemical Company

Tracy Young is the Core R&D Program Director for the Consumer and Infrastructure Solutions Division at The Dow Chemical Company. In this role, she is responsible for leading the innovation portfolio for Energy & Water, Electronic Materials, Building & Construction, Coatings, and Consumer Care. Prior to this role, she was the Growth Technologies R&D Director for the Dow Water and Process Solutions business unit. She is a member of the Dow Corporate Water Strategy Team, and has been actively involved in leading technology programs to address the water-energy nexus and advance Dow's 2025 sustainability goal to advance a circular economy through breakthrough water reuse partnerships. She is currently the co-chair for AIChE's International Society for Water Solutions and past advisory board member for several water industry and research organizations.

During her tenure with Dow, Young has led product and application development across a wide variety of market segments in the plastics and chemicals businesses within biocides, specialty packaging, and performance plastics. She has over 10 years of technical and market leadership team experience with multiple product launches into new markets and a proven track record for driving new innovation growth. In 2009, she led the launch of Dow's new CONTINUUM™ EP HDPE platform and Dow's entry into the caps and closures market as the Rigid Packaging TS&D leader. Young was a member of the Polystyrene Value Center Team and led the establishment of the technical organization for Americas Styrenics LLC in 2008. Within Specialty Packaging, Young led the Films Process R&D group and provided TS&D leadership to the Medical and Wire & Cable market teams to grow barrier films for medical applications and adhesive film metal laminates for fiber optic cable applications. From 1993-2000, Young led developments within Biocides R&D and TS&D to support the adhesives, coatings, personal care, and water treatment markets.

Young earned her Bachelor of Science degree in Chemical Engineering from Michigan State University in 1993. In 2011, she completed training for Executive Leadership through the Broad College of Business at Michigan State University. She is a member of the American Institute of Chemical Engineers with past leadership roles and is currently a member of the Sustainable Engineering Forum. Young has held numerous industry leadership committee roles and active in industry conference presentations, publications, and holds three patents for new commercialized technology.

ICOSSE ’18 Speaker Biographies

Subhas Sikdar, U.S. Environmental Protection Agency (retired)

Dr. Subhas K. Sikdar, now retired, was the Associate Director for Science for the National Risk Management Research Laboratory of the U.S. EPA in Cincinnati, Ohio until 2015. Before joining EPA in 1990, Dr. Sikdar held managerial positions at the National Institute of Standards and Technology in Boulder, Colorado, and General Electric Corporate Research & Development Center in Schenectady, New York. Dr. Sikdar earned his M.S. and Ph.D. in chemical engineering from the University of Arizona. Dr. Sikdar is a Fellow of the American Association for the Advancement of Science (AAAS), Fellow of American Chemical Society (ACS), Fellow of the American Institute of Chemical Engineers (AIChE), Honorary Fellow of the Indian Institute of Chemical Engineers (IIChE), winner of five EPA bronze medals, two R&D 100 awards , AIChE’s Van Antwerpen Service to the Institute Award, AIChE’s Larry Cecil Award for Environmental Chemical Engineering, AIChE’s Sustainability Achievement Award, Distinguished Professional Service Award from EPA, and Distinguished Engineering Alumnus Award from both University of Arizona and University of Calcutta. He served as a member of the Board of Governors of the Council for Chemical Research (CCR) and of the Green Chemistry Institute. He served as the Founder/Chair of Sustainable Engineering Forum, Chair of Institute of Sustainability, and Chair of the Engineers’ Forum for Sustainability (ESF). For 25 years he championed the concepts and methods for clean products and processes for the Agency, in NATO projects, and in various engineering workshops that he organized. He is the founder and the co-Editor-in-Chief of the international journal, Clean Technologies and Environmental Policy (Springer), and served as the section Editor of Current Opinions in Chemical engineering2011-2014 (Elsevier). Currently he is a member of the steering committee of Engineering Conferences International (ECI). Dr. Sikdar has published more than 100 technical papers in reputed journals, has 27 U.S. patents, and has edited 16 books including as a section editor of Encyclopedia of Sustainable Technologies (Elsevier, 2017). His contribution to scientific sustainability, Measuring Progress towards Sustainability, was published as a book by Springer in 2016.

Keynote Speakers

Andrew Mangan, Business Council for Sustainable Development

Andrew Mangan is founder and president of Pathway21, a company that enables business-to-business industrial reuse through the award-winning Materials Marketplace software platform, supporting a culture shift to a circular, closed-loop economy.

Mr. Mangan is also founder and executive director of the United States Business Council for Sustainable Development, a non-profit association of businesses launched in 1993. The Council combines the capabilities of its members to develop, test and scale sustainability solutions.

The Materials Marketplace is scaling after more than 20 years of work. It is driven by expert facilitators who help companies upload materials, find reuse opportunities, bring the parties together, and work toward a deal. It also facilitates communication between senior government decision makers and company operators, helping uncover barriers and opening the door to sound solutions.

Mr. Mangan received a master’s degree from the Columbia University Graduate School of Journalism and joined the Columbia School of International Affairs as an International Fellow. Prior to launching the Business Council, he served as deputy commissioner for natural resources with the Texas General Land Office, as a congressional correspondent for the Associated Press, and as a commercial salmon fisherman in Southeast Alaska.

Heriberto Cabezas, U.S. Environmental Protection Agency and Pazmany Peter Catholic University

Heriberto Cabezas serves as Senior Science Advisor to the Land and material Management Division in the U.S. EPA's Office of Research and Development (ORD), and Research Professor at the Institute for Process Systems Engineering and Sustainability at the Pazmany Peter Catholic University in Hungary. His wards include: 1998 U.S. EPA Science Achievement Award in Engineering, 2007 Distinguished Alumni Achievement Award from the New Jersey Institute of Technology, 2011 Research Excellence Award in Sustainable Engineering from the AIChE, ORD Sustainability Award (team) from the U.S. EPA, 2013 Lawrence K. Cecil Award in Environmental Chemical Engineering from the AIChE. Dr. Cabezas holds a Ph.D. from the University of Florida in thermodynamics and statistical mechanics, a M.S. from the University of Florida, and a B.S. (magna cum laude) from the New Jersey Institute of Technology, all in chemical engineering. He served as Embassy Science Fellow at the U.S. Embassy in Zagreb, Croatia for March - April 2014. His publications include over eighty peer-reviewed articles. He is a Fellow of the AIChE, a member of the American Association for the Advancement of Science, and a Board Certified Member of the American Academy of Environmental Engineers and Scientists. Dr. Cabezas' current research interests focus on: (1) the design of sustainable chemical processes and supply chains, (2) the design of sustainable productions systems in the nexus of food-energy-water, and (3) the development of resilience and reliability criteria for industrial systems.

Bhavik Bakshi, Ohio State University

Bhavik Bakshi is a Professor of Chemical and Biomolecular Engineering at The Ohio State University. He also holds appointments in Civil, Environmental and Geodetic Engineering at OSU and as a Visiting Professor at the Indian Institute of Technology in Mumbai, India. His research is developing methods and applications for assessing and designing sustainable systems that respect nature's limits and reduce the chance of unintended harm. He received his chemical engineering degrees from the University of Bombay and the Massachusetts Institute of Technology, with a minor in technology and environmental policy from MIT and Harvard.

Michael A. Schultz, PTI Global Solutions

Mike Schultz is Managing Director of PTI Global Solutions, with scale-up expertise in the fuels, chemicals, and sustainability space, leading the scale up and commercialization of a number innovations to improve existing technology and get breakthrough technology to the market. He has extensive international experience with postings in Malaysia and New Zealand, and frequent travel throughout his career supporting partners and customers in China, India, Japan, Korea, Russia, SE Asia, and Europe

ICOSSE '18 Speaker Biographies

Michael Gromacki, Dixie Chemical

Mr. Michael Gromacki serves as President of Dixie Chemical. He has over 25 years of experience in the chemical industry. He started his career in engineering consulting practice and joined TOTAL S.A. subsidiary Cook Composites & Polymers (CCP) in 1997 where he served for twelve years in a progression of roles leading to Vice President. He joined Dixie Chemical in March of 2009 as Vice President of Operations and added the role of Chief Technology Officer in 2010. He was promoted to Senior Vice President in July 2014 and in June 2015, he assumed the leadership of Dixie. He was appointed as President in March 2016. He is a Chemical Engineering graduate of University of Wisconsin. He serves on the Boards of the American Composites Manufacturers Association (ACMA), the American Coatings Association (ACA), the National Association of Manufacturers (NAM), the Texas PACE Authority, and the US Business Council for Sustainable Development (USBCSD).

Emily Tipaldo, American Chemistry Council

Emily Tipaldo is Director of Packaging & Consumer Products, at the American Chemistry Council's Plastics Division.

Emily leads the Plastics Division's Packaging Team, representing major U.S. resin suppliers. She directs advocacy and develops strategies for policies and initiatives that recognize plastic packaging and plastic products as valuable resources. Emily leads the Packaging Team in the quest for sustainable solutions for creating and recovering plastics, keeping molecules in play, and, preventing marine debris. As Director, she executed the first natural capital accounting study for the plastics industry, and regularly presents to product manufacturers, brands, and NGOs. She also manages the Materials Recovery for the Future flexible plastic packaging recycling research – representing the flexible plastic packaging value chain, including Fortune 100 companies.

Emily was recently featured as part of the Edison Awards Women Behind Innovation series (September 2017), and was named a Plastics News Rising Star in 2015. Prior to joining the Plastics Division, Emily was Director of Regulatory and Technical Affairs at ACC. Emily received a B.A. (cum laude) in American Studies from Mary Washington College, and a M.A. in International Relations (With Distinction) from the University of Westminster, London.

Panel: Sustainability by Manufacturing USA Institutes

Haresh Malkani, Clean Energy Smart Manufacturing Innovation Institute (CESMII)

Haresh was appointed CTO of CESMII starting March 1, 2018. He brings over 29 years of experience in an industrial RD&E environment covering development and deployment of Smart Manufacturing technologies including sensing, automation, control, modeling, simulation and analytics for applications in continuous, hybrid and discrete manufacturing operations.

In his role as CTO for CESMII, Haresh oversees the technology mission, road map and objectives of CESMII. He will spearhead development of technologies spanning advanced sensors, controls, platforms, data analytics, modeling for manufacturing, and smart manufacturing standards and protocols. He will oversee the development and application of the nation's first open, collaborative Smart Manufacturing technology platform for industrial applications. In addition, he will provide guidance on the institute's technical program content for training and workforce development.

Prior to joining CESMII, Haresh was Director of Digital Manufacturing & Automation Technologies at Arconic/Alcoa. Haresh was responsible for developing the strategy for Smart Manufacturing and deploying solutions that drove productivity across the company's discrete and hybrid operations. His expertise in modeling, simulation, advanced sensing, automation, analytics and visualization were key to developing the technical strategy, architecture and approach. Haresh has a successful history of projects developing model-based process control and simulation systems for several unit operations at Arconic/Alcoa.

In addition, Haresh has been involved with the Smart Manufacturing Leadership Coalition (SMLC) for over 8 years and recently held the position of Vice Chairman of SMLC.

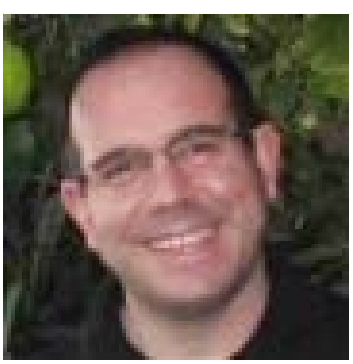
Haresh holds a Ph.D. and MS in Mechanical Engineering from Northwestern University, Illinois and a B.E. Mechanical Engineering from Maharaja Sayajirao University, India.

Nabil Nasr, REMADE Institute

Dr. Nabil Nasr is the founding Chief Executive Officer of the REMADE Institute, where he oversees everything from node-level research roadmap development to corporate engagement of the Institute's largest industrial partners. Dr. Nasr also serves as the Director of the Golisano Institute for Sustainability and an Associate Provost for Academic Affairs at the Rochester Institute of Technology. Throughout his career, Dr. Nasr has worked in the fields of sustainable manufacturing, remanufacturing, clean production, and sustainable product development for over 25 years, and is considered an international leader in research and development efforts in those disciplines. Dr. Nasr has served as an expert delegate for the U.S. government in several international forums, including the Asia Pacific Economic Cooperation (APEC), the United Nations, the World Trade Organization (WTO), and the Organisation for Economic Cooperation and Development (OECD). Dr. Nasr is also a member of the International Resource Panel (IRP) of the United Nations Environment Programme (UNEP). Dr. Nasr's significant expertise in sustainable manufacturing leadership continues with his latest endeavor, the REMADE Insitute.

Dr. Nasr holds a BS in Industrial Engineering from Helwan University (Egypt), an MEng in Manufacturing Engineering from the Pennsylvania State University, and both an MS and PhD in Industrial & Systems Engineering from Rutgers University.

Ignasi Palou-Rivera, RAPID Manufacturing Institute



Ignasi Palou-Rivera is the Technical Program Manager of the RAPID Manufacturing Institute, a part of the American Institute of Chemical Engineers (AIChE). The RAPID Institute focuses in the promotion of modular chemical process intensification (MCPI) with the goal of reducing the capital and energy intensity of the US process industries.

Ignasi holds a Ph.D. in Chemical Engineering from the University of Wisconsin-Madison, and an Engineer Degree from the Universitat Politècnica de Catalunya in Barcelona. His technical background spans the areas of process modeling and optimization, techno-economic and life-cycle and sustainability analysis of fuels and chemicals, and R&D management. He has been a part of a variety of industrial and academic organizations such as LanzaTech (a renewable fuels and chemicals start-up with a proprietary gas fermentation technology), Argonne National Laboratory, BP Refining Technology, Aspentech, etc.

Ignasi is a Senior Member of AIChE, and has been heavily involved in volunteer positions with CAST Division (Computing & Systems Technology Division) as well as being the current Chair of the Sustainable Engineering Forum (SEF).

Presentation Instructions for ICOSSE '18

Oral Presentations

Please check the Technical Program for your scheduled presentation time - speaking slots are 18 minutes (including Q&A) for selected speakers, 35 for Keynote speakers and 45 minutes for Plenary speakers (please check the schedule). Presentations should be in PowerPoint format and should be uploaded to the projection computer at least 15 minutes prior to the start of your session.

Poster Presentations

Poster Session

- The Poster Session will be held on Monday, August 13 afternoon directly after the Rapid Fire Session. Please put your posters up as soon as you arrive on Sunday afternoon to display your poster during the Opening Reception.

- Poster presenting authors are responsible for printing, setting up and taking down their poster; mounting supplies will be provided.

- The poster board surface will be 30 x 40 inches, portrait or landscape – please do not print your poster any bigger.

- There will be an ICOSSE Student Poster competition – undergraduate and graduate students will be interviewed by ICOSSE judges during the ICOSSE Poster Session. Winners will be announced the following day during the ICOSSE Awards and Closing Remarks.

Rapid Fire Poster Session

- All Poster presenters are invited to participate in the ICOSSE Rapid Fire Session, where the author will display one slide (PPT, 16:9, no animations) and in 90 seconds or less present the key information about their poster to the conference audience. You may use your Poster as the slide. The Rapid Fire presentation is meant to be an abstract rather than a comprehensive explanation of your work. The complete explanation should be reserved for the poster session.

- There will be a Rapid Fire People's Choice Award competition, where presenters will be judged on content, presentation, and adherence to the time limit by the audience.

- Poster authors wishing to take part in the Rapid Fire session must send their slide by August 12 to lucya@aiche.org or notify me if you do not wish to participate.

Code of Conduct

AIChE Volunteer and Meeting Attendee Conduct Guidelines

AIChE's volunteers are the core of the Institute and make all of its programs, conferences and educational efforts possible. These offerings provide excellent opportunities for AIChE members and meeting attendees to gain greater technical expertise, grow their networks, and enhance their careers. AIChE events provide engineers, scientists, and students a platform to present, discuss, publish and exhibit their discoveries and technical advances.

At all times, volunteers and meeting attendees should act in accordance with AIChE's Code of Ethics, upholding and advancing the integrity, honor and dignity of the chemical engineering profession. AIChE's Board of Directors has developed these guidelines to foster a positive environment of trust, respect, open communications, and ethical behavior. These guidelines apply to meetings, conferences, workshops, courses and other events organized by AIChE or any of its entities and also to volunteers who conduct other business and affairs on behalf of AIChE.

Specifically

1. Volunteers and meeting attendees should understand and support AIChE's Code of Ethics.
2. Volunteers and meeting attendees should contribute to a collegial, inclusive, positive and respectful environment for fellow volunteers and attendees, and other stakeholders, including AIChE staff.
3. Volunteers and meeting attendees should avoid making inappropriate statements or taking inappropriate action based on race, gender, age, religion, ethnicity, nationality, sexual orientation, gender expression, gender identity, marital status, political affiliation, presence of disabilities, or educational background. We should show consistent respect for colleagues, regardless of discipline, employment status, and organizations for which they work, whether industry, academia, or government.
4. Disruptive, harassing or other inappropriate statements or behavior toward other volunteers, members, and other stakeholders, including AIChE staff, is unacceptable.
5. Volunteers and meeting attendees should obey all applicable laws and regulations of the relevant governmental authorities while volunteering or attending meetings. Volunteers and meeting attendees taking part in any AIChE event, including the ChemECar CompetitionTM, should also comply with all applicable safety guidelines.

Violations of this conduct policy should be reported promptly to the AIChE President or Executive Director.

ICOSSE '18 Conference Chairs

Raymond Smith, *U.S. Environmental Protection Agency*
David Shonnard, *Michigan Technological University*
Wendy Young, *Chemstations, Inc.*

Steering Committee

Tracy Young, *The Dow Chemical Company*
Andrew Mangan, *Business Council for Sustainable Development*
Heriberto Cabezas, *U.S. Environmental Protection Agency; Pazmany Peter Catholic University*
Yinlun Huang, *Wayne State University*
Nabil Nasr, *RIT; REMADE Institute*
Peter Saling, *BASF*
Freya Burton, *LanzaTech*

The 7th International Congress on Sustainability Science & Engineering is organized by the AIChE Institute of Sustainability.

AIChE The Global Home of Chemical Engineers

institute for sustainability
An AIChE Technological Community