



# ICOSSE'20

International Congress on Sustainability Science & Engineering

### AUGUST 3-5, 2020



Organized by the Institute for Sustainability

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### WELCOME ADDRESS

### Welcome!

We would like to personally welcome you to the virtual 9th International Congress on Sustainability Science & Engineering (ICOSSE'20) brought to you by the Institute for Sustainability (IfS), an American Institute of Chemical Engineers (AIChE) technological community, and hosted by vFairs. The world of Sustainability is an exciting and essential area in which to work or study, and the IfS will continue to meet, even virtually, and bring motivated people together in forums like this, to ensure that sustainability research remains at the cutting edge.

ICOSEE'20 serves as the international platform for innovation in sustainability science and engineering to discuss the trends driving Sustainability research and innovation and present the latest in new sustainable process technologies. As part of charting a course forward, this year's Congress will also focus on several topics concerning Sustainability as a whole with session topics providing deeper understanding of critical areas including Biological Sustainability; Material Recycling; and the Circular Economy.

In Sustainability, as elsewhere in the world today, we have a unique opportunity to move from our current state to one of much more profound understanding, as disruption begets change. As global sustainability challenges mount and in the midst of a pandemic that we all are experiencing first-hand, we are in the midst of an extraordinary time. It is an important time for the science and sustainability community to come together in the face of these challenges. The creativity, ingenuity, and care that sustainability scientists and engineers have shown as we banded together while being apart have kept the essence, authenticity, and spirit of progress alive and well, providing inspiration for the progress highlighted in this year's Congress.

Much work has gone into making this conference a success. We extend deep-felt gratitude to the members of the expert Steering Committee for their contributions, and to AIChE's excellent meetings staff for making it possible to hold the Congress under the unusual circumstances. We would also like to thank each of the distinguished speakers and panelists who made this conference possible.

Our thanks, also, to each of you for attending this year's Congress and bringing your expertise to this gathering. Throughout this conference, we ask you to stay engaged, be proactive, and help to shape the future of the world through sustainability initiatives. Our respect and thanks go out to all of you, and we trust that your experience will be a pleasant, educational, and inspiring one.

### Sincerely, ICOSSE'20 Conference Chairs

**Eric C. D. Tan** National Renewable Energy Laboratory Golden, Colorado, USA



Anne Johnson Resource Recycling Systems Ann Arbor, MI



David Thompson Idaho National Laboratory, Idaho Falls, Idaho, USA



### **CONFERENCE ORGANIZERS**

### Conference Organizers and Sponsors

### Organizing Committee

Bhavik Bakshi, Ohio State University Birdie Carpenter, National Renewable Energy Laboratory Yinlun Huang, Wayne State University Chad King, University of Denver Amy E. Landis, Colorado School of Mines Lise Laurin, Earthshift Global Kristin C. Lewis, CAAFI Silvia Palma-Rojas, California Energy Commission Timothy G. Rials, University of Tennessee Gerardo Ruiz-Mercado, US EPA Jeff Seay, University of Kentucky Raymond Smith, US EPA

Sponsors





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### **TECHNICAL PROGRAM**

### Technical Program

Day 1: Monday, August 3<sup>rd</sup>

10:00 AM	10:10 AM	Introduction to Day 1
10:10 AM	10:40 AM	Leveraging Sustainability Regarding Plastic: Law and Policy Landscape; Keynote Speaker - Mary Ellen Ternes, Earth and Water Group
10:40 AM	11:20 AM	Sustainable Supply Chains (logistics management)
11:20 AM	11:30 AM	Competition of Renewable Feedstocks
11:30 AM	11:40 AM	Bio-Restore: Biomass to Restore Natural Resources
11:40 AM	12:10 PM	Question and Answer Panel featuring Speakers from: Sustainable Supply Chains (logistics management) Competition of Renewable Feedstocks Bio-Restore: Biomass to Restore Natural Resources
12:10 PM	12:15 PM	Break
12:15 PM	12:45 PM	Meet and Greet with ICOSSE
12:45 PM	12:50 PM	Break
12:50 PM	1:40 PM	Biomass Conversion Technologies (Part 1)
1:40 PM	1:45 PM	Break
1:45 PM	2:30 PM	Biomass Conversion Technologies (Part 2)
2:30 PM	3:10 PM	Question and Answer Panel featuring Speakers from: Biomass Conversion Technologies
3:10 PM	3:40 PM	Short Presentations
3:50 PM	4:45 PM	Modeling and Simulation
4:45 PM	5:15 PM	Question and Answer Panel featuring Speakers from: Modeling and Simulation
5:15 PM	5:30 PM	End of Day 1 Summary by the Chairs



### **TECHNICAL PROGRAM**

### Day 2: Tuesday, August 4<sup>th</sup>

Day 2: Recycli	ing and Beyond	
10:00 AM	10:10 AM	Introduction to Day 2
10:10 AM	10:40 AM	A Big Picture Treatise to Sustainable Development and Innovation,
		Keynote Speaker - Minal Mistry, Oregon DEQ
10:45 AM	11:55 AM	Design for Circularity
11:55 AM	12:20 PM	Question and Answer Panel featuring Speakers from:
		Design for Circularity
12:20 PM	12:25 PM	Break
12:30 PM	12:50 PM	End-of-Use (Life) of goods (products)
12:50 PM	1:25 PM	Waste to Energy (fuel or power)
1:25 PM	1:50 PM	Question and Answer featuring Speakers from:
		End-of-Use (Life) of Goods (Products)
		Waste to Energy (Fuel or Power)
1:50 PM	2:00 PM	Break
2:05 PM	2:55 PM	Advanced Recycling Technologies
2:55 PM	3:20 PM	Question and Answer featuring Speakers from:
		Advanced Recycling Technologies
3:20 PM	3:25 PM	Break
3:30 PM	4:05 PM	Waste Valorization (plastics and more)
4:05 PM	4:30 PM	Question and Answer featuring Speakers from:
		Waste Valorization (Plastics and More)
4:30 PM	4:40 PM	End of Day 2 Summary by the Chairs
4:40 PM	5:00 PM	Happy Hour + Icebreakers



### **TECHNICAL PROGRAM**

Day 3: Sustain	ability and More	
10:00 AM	10:10 AM	Introduction to Day 3
10:10 AM	10:30 AM	Sustainable Process Design and Manufacturing
10:30 AM	11:00 AM	Sustainable Social-Ecological Systems
11:00 AM	11:10 AM	Innovation for Sustainable Businesses and Industries
11:10 AM	11:40 AM	Live Question and Answer Panel featuring Speakers from:
		Sustainable Process Design and Manufacturing
		Sustainable Social-Ecological Systems
		Innovation for Sustainable Businesses and Industries
11:40 AM	11:45 AM	Break
11:45 AM	12:15 PM	Discussion Break Out Session
12:15 PM	1:00 PM	Decarbonization
1:00 PM	1:20 PM	Question and Answer featuring Speakers from:
		Decarbonization
1:20 PM	1:25 PM	Break
1:25 PM	2:05 PM	Renewable/Alternative Energy
2:05 PM	2:20 PM	Question and Answer featuring Speakers from:
		Renewable/Alternative Energy
2:20 PM	2:50 PM	Short Presentation- Posters
2:50 PM	2:55 PM	Break
2:55 PM	3:35 PM	Nutrient Pollution, Prevention, and Control
3:35 PM	3:55 PM	Food, Energy, Water Nexus
3:55 PM	4:25 PM	Question and Answer featuring Speakers from:
		Nutrient Pollution, Prevention and Control
		Food, Energy, Water Nexus
4:25 PM	4:30 PM	End of Conference: Conclusions and Next Steps from the Chairs

### Day 3: Wednesday, August 5<sup>th</sup>



### **Keynote Speakers**



### MARY ELLEN TERNES

#### Earth & Water Law, LLC

Mary Ellen Ternes is a partner in the Oklahoma City office of D.C. based Earth & Water Law, LLC. Ms. Ternes represents energy, manufacturing and other industrial and municipal clients, with in-depth experience in air, hazardous waste, wastewater, drinking water program permitting, compliance, with particular emphasis in developing efficient regulatory strategies for complex and high profile processes and industries, enforcement defense, risk management, due diligence, voluntary cleanup practices as well as federal and state rulemaking, administrative proceedings and litigation. Ternes began her career as a chemical engineer for the U.S. EPA Region 6 in Superfund emergency response and RCRA hazardous waste incinerator permitting, then left EPA to join industry, managing environmental compliance for a commercial hazardous waste incineration company, negotiating air, hazardous waste, and toxic substances treatment and disposal permits, demonstrating compliance and conducting audits.

#### MINAL MISTRY

#### Oregon Department of Environmental Quality

Minal Mistry is the business initiatives lead with the Oregon DEQ (Department for Environmental Quality). He works with a wide range of entities to implement strategies for Oregon's 2050 Vision for Materials Management. His primary focus is on helping businesses produce and consume materials in more sustainable ways. Minal supports concept development, research, and capacity building in support of the Vision. Minal's professional experiences include life cycle assessment, environmental testing, information services, technical training, and consulting for implementing Design for Environment (DfE) strategies for consumer packaged goods. Minal is a biologist who has worked with varied businesses, environmental NGOs and government.



### Featured Speakers | In order of Session and Appearance

### Sustainable Supply Chains (Logistics Management)

#### **Damon Hartley**

### Idaho National Laboratory

Damon Hartley is the lead of the biomass analysis team at the Idaho National Laboratory, where he and his team provide analysis to inform the economics and sustainability of technological developments along the biomass feedstock supply chain and provide guidance for future research and development needs to enable the development of a bioeconomy. Damon's expertise is in modeling the logistics systems and he primarily focuses on the optimization of transportation networks, simulation of physical systems and techno-economic analysis. Damon received his PhD, from West Virginia University in Forest Resource Management, where he focused on the development, analysis and optimization of woody biomass supply chains in the Northeastern U.S. Prior to receiving his PhD, he served as the statewide extension specialist for Forest Operations for the Ohio State University and as a watershed forester for the State of Maryland's Department of Natural Resources, responsible for a portion of the Chesapeake Bay watershed.

#### Sarang Supekar

#### Argonne National Laboratory

Dr. Sarang Supekar is a staff scientist in the Energy Systems Division at Argonne National Laboratory. He received his Ph.D. in Mechanical Engineering from the University of Michigan. His research is on advanced manufacturing technologies and manufacturing systems that could achieve transformative gains in process productivity and enhance manufacturing sustainability. He also develops optimization and life cycle models analyzing energy technologies and energy and transportation systems of the future. Dr. Supekar's specific areas of interest include (1) process modeling, and data-driven decision making in manufacturing systems; (3) gas-based technologies to mitigate water use and pollution in energy-efficient "dry factories"; (4) life cycle assessment, and techno-economic analysis of carbon capture and utilization pathways; and (5) optimization and simulation models for technology forecasting for a low-emissions energy future.

#### **Philip Tominac**

#### University of Wisconsin – Madison

Philip Tominac is a postdoctoral researcher in Victor Zavala's research group in the Department of Chemical and Biological Engineering at the University of Wisconsin - Madison. He received his PhD in Chemical Engineering from McMaster University under the supervision of Vladimir Mahalec, studying competitive interactions in supply chains. Philip is interested in multi-stakeholder network models and supply chain optimization. He is currently working on market models for environmental policy design.

### Competition of Renewable Feedstock

#### **VeeAnder Mealing**

#### Colorado School of Mines

VeeAnder Mealing is a 3rd year PhD candidate in the Mines Environmental Engineering program. Her current research is focused on analyzing the sustainability of emerging feedstocks, guar & guayule, to support the development of a sustainable bio-economy in the southwestern U.S. She is from North Augusta, SC and earned her B.S. in Biosystems Engineering and M.S. in Bioengineering from Clemson University. She is passionate about holistic sustainability and serving and supporting underrepresented individuals in STEAM. She enjoys traveling, cooking, and new adventures in nature.

Research

### Bio-Restore: Biomass to Restore Natural Resources

### Michael Griffel

### Idaho National Laboratory

Mike Griffel is a data scientist at the Idaho National Laboratory supporting multiple bioenergy projects. He is the principal investigator for the Integrated Landscape Management project supporting the U.S. Department of Energy's Bioenergy Technologies Office and has extensive experience conducting modeling assessments of economic and environmental outcomes resulting from the integration of bioenergy crops into agricultural landscapes, including evaluation of ecosystem services in Midwest agroecosystems. Prior to joining the lab, he managed a precision agriculture program and provided technical agronomy services to farmers and crop advisors in the Pacific Northwest region.

### Bio-Restore: Biomass to Restore Natural Resources

### **David Lanning**

### Forest Concepts, LLC

Dave Lanning is the senior mechanical engineer for the Forest Concepts, LLC. He received a bachelor's degree in mechanical engineering from the University of Washington in 2003. While at the university, Dave led a senior design project team that worked on more efficient methods to produce Forest Concepts' WoodStraw® products. He has since led Forest Concepts' development of the rotary shearing technology and equipment that is used to manufacture precision feedstock particles at a fraction of the traditional method's energy consumption. Mr. Lanning is an active member of the American Society of Agricultural and Biological Engineers (ASABE). As part of that organization, Dave has chaired the ASE12 Forest Engineering technical committee for multiple terms. Mr. Lanning authored and coauthored numerous conference papers. As part of Dave's research and development efforts with Forest Concepts, he has developed many of their core biomass processing technologies alongside the excellent development team at Forest Concepts. These novel technologies have earned Dave 10 patents as lead inventor and an additional 16 patents as co-inventor.

### Hannah Nguyen

### National Renewable Energy Laboratory

My Ph.D thesis at University of Delaware focused on understanding structure-activity relationships of multifunctional catalysts in tandem reactions for biomass valorization. After joining NREL as a postdoctoral researcher, I continue my research on biomass conversion for fuel application with the focus on catalyst design for raw materials and reactor scale-up.

### Jacob S. Kruger

### National Renewable Energy Laboratory

Dr. Jacob Kruger is a research engineer at NREL and has more than ten years of experience in catalytic processing of lignocellulose and other renewable feedstocks. His current work focuses on conversion of lignin residues and microbial biomass (including algae) to high-value products.

### Pahola Thathiana Benavides

### Argonne National Laboratory

Dr. Benavides studies the energy and environmental effects of conversion processes used to produce fuels and chemicals from bio-based and waste feedstocks. She has also studied catalyst production, their impact on the life cycle of biofuels, and the fate of catalyst waste materials from catalyst production and use. Recently, she has been studying plastic production pathways to quantify the life cycle GHG emissions and fossil fuel consumption of bioplastics, considering end-of-life (EOL) tradeoffs between biodegradability and carbon sequestration. She has worked closely with colleagues at other national laboratories on projects including evaluations of bioproducts and biofuels through the Clean Energy Manufacturing Analysis Center (CEMAC) and ongoing projects thought BETO Co-Optimization of Fuels and Engines (Co-Optima) and Agile BioFoundry (ABF).

### **Andrew Bartling**

### National Renewable Energy Laboratory

Andrew W. Bartling is a process engineer in the Economics, Sustainability, and Market Analysis team at the National Renewable Energy Laboratory (NREL) where he focuses on process design, simulation, and technoeconomic analysis (TEA) of biorefineries producing bio- fuels and products from lignocellulosic biomass feedstocks. Andrew's current research interests include TEA of biofuels produced via biochemical and thermochemical conversion routes, feedstock variability impacts on biorefinery economics, and strategies for reducing production costs of fuels and chemicals produced from lignin.

### **Art Ragauskas**

### Oak Ridge National Laboratory

Arthur Ragauskas held the first Fulbright Chair in Alternative Energy and is a Fellow of American Association for the Advancement of Science, the International Academy of Wood Science and TAPPI. In 2014, he assumed a Governor's Chair for Biorefining based in University of Tennessee's Department of Chemical and Biomolecular Engineering, with a complementary appointment in the UT Institute of Agriculture's Department of Forestry, Wildlife, and Fisheries and serves in the Energy and Environmental Sciences Directorate, Biosciences Division, at ORNL. His research program is directed at understanding and exploiting innovative sustainable bioresources. This multifaceted program is targeted to develop new and improved applications for nature's premiere renewable biopolymers for biofuels, biopower, and bio-based materials and chemicals. His research program has been sponsored by NSF, USDA, DOE, GA Traditional Industry Program, a consortium of industry partners, and several fellowship programs which is summarized in 535 publications. His Fulbright sponsored activities at Chalmers University of Technology, Sweden were focused on the forest biorefinery and new biofuel conversion technologies for lignocellulosics. Currently, Dr. Ragauskas manages a research group of graduate students, postdoctoral research fellows, a research scientist, and visiting scientists. He is the recipient of the 2014 TAPPI Gunnar Nicholson Gold Medal Award, the 2014 ACS Affordable Green Chemistry Award, 2017 AIChE Green Processing Award, 2017 Academia Distinguished Service Award, 2019 AIChE Chase Award, and his students and postdocs have won several awards, including the ACS graduate research award, ORNL UT-Battelle Award, and the ORNL Supplementary Performance Award

### **Nicholas E. Thornburg**

### National Renewable Energy Laboratory

Dr. Nicholas (Nick) Thornburg is a Chemical Reaction Engineer at the National Renewable Energy Laboratory (NREL), where he studies routes to renewably-sourced chemicals and transportation fuels as well as the fuel efficiency of modern engines. Nick has a B.S. in Chemical Engineering from Washington University in St. Louis and a Ph.D. in Chemical Engineering from Northwestern University, in addition to industrial R&D experience with the Dow Chemical Company and 3M.

### **Xiangchen Huo**

### National Renewable Energy Laboratory

Dr Xiangchen Huo is a Chemical Engineering Postdoctoral Researcher at the National Renewable Energy Laboratory (NREL). Her current research focuses on the development of catalysts and processes for the upgrading of biological and pyrolysis intermediates to renewable gasoline, diesel, and aviation fuels. She also has research interests in water treatment technologies including oxidation, reduction, and membrane separation. She received a B.S. and M.S. from Tongji University in Shanghai, China, and a Ph.D. in Civil and Environmental Engineering from the Colorado School of Mines in Colorado, US.

### Mark R. Nimlos

### National Renewable Energy Laboratory

The development and deployment of renewable carbon-based transportation fuels, chemicals, and materials is critical to sustainability, energy security, and continued economic growth. Dr. Mark R. Nimlos' research interests are focused on using thermochemistry to facilitate biomass as a source of renewable carbon, helping grow the bioeconomy. Increasing the use of renewable, biomass-sourced carbon will require developing science and

technology for conversion into useful products and demonstrating the performance of these products in existing and future applications. During his 31-year career at NREL, Dr. Nimlos has worked on pyrolysis, gasification and catalytic fast pyrolysis as conversion technologies to produce biofuels, which are a sustainable, inexpensive energy source for transportation. To facilitate the economics of biorefineries that would produce biofuels, he has recently focused his research efforts on producing chemical and material co-products from these biofuel conversion processes. Developing uses for these coproducts will help improve the economic resilience of biorefineries and will improve the sustainability of plastics and other carbon-based materials.

### Modeling and Simulation

### Fernando V. Lima

### West Virginia University

Fernando V. Lima joined the faculty as an Assistant professor of Chemical Engineering at West Virginia University (WVU) in January 2013. He is now an Associate Professor of Chemical Engineering since August 2019. His research group at WVU focuses on the development and implementation of process systems engineering methods for process design and intensification, advanced control and state estimation, modular energy systems and sustainability. He received his B.S. degree from the University of São Paulo in 2003 and his Ph.D. from Tufts University in 2007, both in Chemical Engineering. Upon completion of his Ph.D., he was a research associate at the University of Wisconsin-Madison and a postdoctoral associate at the University of Minnesota. Dr. Lima has served as the AIChE Society Associate Editor for the American Control Conference (ACC) for five years (2013-2015, 2017-2018). He is also a guest editor for Special Issues of Processes and Industrial and Engineering Chemistry Research journals and a member of the Editorial Boards of Journal of Process Control and Processes.

### Noah Sandoval

### Colorado School of Mines

Noah Sandoval graduated from Colorado State University in 2013 with a degree in Engineering Education and Spanish. Following his undergraduate experience he spent a year at La Universidad Autónoma de Yucatán teaching introductory engineering and advanced English courses. Following this he joined Teach For America and taught high school science for five years in Oklahoma and then in Denver. He started the Advanced Energy System Master's Program at Colorado School of Mines in the fall of 2019 and was accepted to the Ph.D. Program in the spring of 2020. His research goals are to improve the energy efficiency of buildings with a focus on retrofitting, life cycle assessment, and social equity.

### **Emmanuel A. Aboagye**

### Rowan University

Emmanuel A. Aboagye received his Bachelor of Science in Chemical Engineering from Kwame Nkrumah University of Science and Technology, Ghana. Currently, he is a Ph.D. student under the supervision of Dr. Kirti M. Yenkie at Rowan University, NJ, USA. My research interests include the systematic design and sustainability assessment of environmental remediation processes using computational tools.

### **Carrie Hartford**

### Jenike and Johanson

Carrie Hartford, Technical Sales Manager, and Senior Project Engineer has been with Jenike and Johanson for over a decade designing bins, silos, feeders, and transfer chutes to solve challenging material handling problems for clients in all industries. She teaches courses, writes papers, and gives technical presentations all over the world regarding the science of bulk solids handling and storage. She holds a Mechanical Engineering degree, MBA, and California Professional Engineers license. Carrie is based out of San Luis Obispo, California – previously she established Jenike & Johanson's office in Perth Australia.

#### Rebecca Hanes

#### National Renewable Energy Laboratory

Rebecca Hanes is a Modeling and Analysis Engineer in the Strategic Energy Analysis Center at the National Renewable Energy Laboratory. She uses a variety of modeling techniques to assess the sustainability of large-scale agricultural and industrial systems and builds decision support tools to inform the sustainable design and operation of such systems.

### **Design for Circularity**

#### **Melissa Bilec**

### University of Pittsburgh

Dr. Melissa Bilec is an associate professor in the Swanson School of Engineering's Department of Civil and Environmental Engineering; she is the Deputy Director of the Mascaro Center for Sustainable Innovation. She is also the Roberta A. Luxbacher Faculty Fellow, and she serves as the Pitt STRIVE Director of Faculty Community Building and Engagement for Diversity, Equity, and Inclusion. Bilec's research focuses on the sustainable built environment. She explores system-level environmental performance of buildings, while developing a deeper understanding of environmental impacts, energy use, and indoor air quality. She is an expert in life cycle assessment (LCA), and works to advance LCA through method development. Dr. Bilec is personally interested in high-impact research that addresses significant societal challenges through innovative research approaches. Most recently, she is working to solve the global plastic waste challenge through the advancement and development of circular economy principles.

#### Mi Li

#### University of Tennessee

Dr. Mi Li is an Assistant Professor in Biorefinery and Biopolymer Chemistry at the Center of Renewable Carbon, Department of Forestry, Wildlife, and Fisheries, University of Tennessee Knoxville. Dr. Li earned his doctorate in Wood Science from Auburn University in 2014, and his B.S. and M.S. in Chemical Engineering of Forestry Bioproducts and Biomaterials from Northeast Forestry University in China. After graduation with his PhD, Dr. Li joined the US DOE-funded BioEnergy Science Center at Oak Ridge National Laboratory and The University of Tennessee Knoxville as a post-doctoral research fellow. He primarily worked on lignocellulose (cellulose, hemicellulose, and lignin) recalcitrance and fractionation, chemistry, and characterization for the production of bioenergy, biofuels, and bioproducts. Dr. Li has contributed to about 60 peer reviewed journal publications. He is the recipient of Distinguished Achievement Award 2017 at Oak Ridge National Laboratory and his research has been highlighted at the US DOE Office of Sciences webpage.

### **Peter Canepa**

### Oregon Department of Environmental Quality

Peter Canepa provides Life Cycle Assessment (LCA) expertise to Oregon DEQ's Materials Management program. Peter's primary role is to conduct and support projects that advance Oregon towards achieving its 2050 vision, through the application of LCA. Prior to this role, Peter spent 8 years with Thinkstep, a consultancy specializing in LCA. Peter holds a Master's degree in Environmental Science and Management and a Bachelor's degree in Environmental Studies.

### Vikas Khanna

### University of Pittsburgh

Dr. Vikas Khanna is an Associate Professor and Wellington C. Carl Faculty Fellow in the Department of Civil and Environmental Engineering at the University of Pittsburgh with secondary appointment in Chemical and Petroleum Engineering. Dr. Khanna received his PhD and MS from the Ohio State University, and a BS from Panjab University, all in Chemical Engineering. Before joining Pitt, he was an Associate Engineer in the Biofuels Research and Development group at ConocoPhillips. His research and teaching interests are in the areas of sustainability science and engineering, life cycle assessment of emerging technologies, and modeling of complex systems. His current research focuses on the development of systems-level methods and techniques for understanding the

environmental sustainability of engineered systems and products. Applications include emerging biofuel technologies, management of shale gas produced water, food-energy-water nexus, and quantification of ecosystem goods and services.

#### Julien Walzberg

#### National Renewable Energy Laboratory

Julien Walzberg is a postdoctoral researcher at the National Renewable Energy Laboratory (NREL) (Colorado) and is also an attendee of the Ellen Macarthur Foundation "From linear to circular" program. His current research focuses on modeling socio-technical systems in the context of the circular economy.

### End-of-Use (Life) of goods (products)

### Jose D. Hernandez-Betancur

### US EPA

Jose has a bachelor's degree in chemical engineering, and a master's in materials and processes engineering from the Universidad Nacional de Colombia, Medellin, Colombia. During his master's degree, he worked on a framework for assessing hot-dip galvanizing process sustainability to obtain insights for process engineers and other stakeholders. Currently, Jose is part of an internship program at the Office of Research & Development (ORD), U.S. Environmental Protection Agency. He is pursuing his doctoral degree at Universidad de Salamanca, Spain. As a result of the synergy between both entities, Jose is developing a data-driven framework for supporting chemical risk evaluation at the end-of-life stage.

### Yi Ji

### Purdue University

Yi Ji is a Ph.D. candidate from Environmental Ecological Engineering (EEE) program at Purdue University. She is coadvised by Dr. Fu Zhao and Dr. Chad T. Jafvert. She received her M.S. degree from EEE program at Purdue in 2019. Her research mainly focuses on cathode materials sustainable recovery from spent lithium-ion batteries in electric vehicles and fluoride pollution reduction during recycling process. She is currently involved in projects funded by Critical Materials Institute (CMI). Yi is responsible for improving metal recovery efficiency, analyzing emissions during recycling, and evaluating characteristics of final products.

### Waste to Energy (fuel or power)

### **Derek Vardon**

### National Renewable Energy Laboratory

Derek Vardon is a Senior Staff Research Engineer and research project team leader at the National Renewable Energy Laboratory (NREL). His research interests include applied catalysis for renewable diesel and aviation fuels, fuel-property informed process design, decarbonization of the transportation sector, and advanced catalyst material synthesis and characterization for biomass conversion. Since 2013, he has worked in the National Bioenergy Center at NREL. He received his B.S. (2010), M.S. (2012), and Ph.D. (2015) in Environmental Engineering from the University of Illinois at Urbana-Champaign. Prior to entering college, he served 6 years in the U.S. Navy as a nuclear electrician's mate.

### Mark A. Paisley

### Taylor Biomass Energy, LLC

Mr. Paisley joined Taylor Biomass Energy as the Vice President of Research and Development in August of 2005. He is internationally recognized as an expert in gasification technologies, specializing in biomass gasification. He is the inventor of the Taylor Gasification process and inventor or co-inventor of several other gasification technologies including the SilvaGas<sup>®</sup> process. Mr. Paisley was in charge of the initial development of a major biomass gasification process at Battelle Memorial Institute. Mr. Paisley served as the Vice President for Technology at FERCO Enterprises prior to his employment at Taylor Biomass Energy. Prior to FERCO, he completed a 20-year career at Battelle, and worked at Bituminous Coal Research and the Babcock & Wilcox Research Center.

Mr. Paisley has over 48 years of experience with gasification technologies and energy and chemical value recovery from fuel and residue materials. He has extensively published articles relating to biomass gasification and fuel conversion technologies. As an expert in the renewable energy field, Mr. Paisley authored the Biomass Energy section for the online Kirk-Othmer Encyclopedia of Chemical Technology.

holds several U.S. and foreign patents on energy and material recovery processes. In 1998, Mr. Paisley was awarded the R&D 100 Award for the SilvaGas<sup>®</sup> gasification process.

### **Mohammed Awwad**

### King Fahad University of Petroleum and Minerals (KFUPM)

Mohammed Awwad is a junior chemical engineering student and minor in chemistry at King Fahad University of Petroleum and Minerals (KFUPM). He has been actively involved in the undergraduate research for the last two years. Mohammed is an enthusiastic student with ample appetite for research and innovation. At the sophomore year, he had been working for a year in Research Institute (RI) trying to develop a novel electrocatalyst employed to produce Hydrogen (H2) from water and he participated as co-author in a published scientific paper. One year ago, he had been working on the chemical recycling of plastics wastes, particularly on the modeling and simulation of pyrolysis and gasification. His work focused on the technical and economic factors that can improve the cost competitiveness of the recycled plastics. After graduation, Mohammed wishes to pursue higher degree in one of the reputable universities aiming to apply his knowledge as chemical engineer in order to make a positive change in our world.

### Advanced Recycling Technologies

### **Brian Davison**

### Oak Ridge National Laboratory

Brian H. Davison is Chief Scientist for Systems Biology and Biotechnology, Oak Ridge National Laboratory and is Chief Science Officer in the DOE Center For Bioenergy Innovation (cbi.ornl.gov). He has 170+ publications and 15 patents in bioprocessing, industrial microbiology, biofuels and bioproducts. His PhD in ChemE. is from California Institute of Technology and BS in ChemE from U of Rochester. He co-chaired the 15th to 26th Symposia on Biotechnology for Fuels and Chemicals. He is on the Board of the Society for Biological Engineering. Honors include an R&D100 for bio-succinic acid, the SIMB CD Scott award, SIMB Fellow and AIChE Fellow.

### Jennifer Le Roy

### **BioCellection Inc.**

Jennifer is the CTO at BioCellection Inc., a chemical recycling start-up that upcycles plastic waste. She currently oversees process development, product development, and scaleup efforts. Her background is in synthetic chemistry and materials science (PhD University of Ottawa, Canada) and she is a co-inventor of BioCellection's proprietary recycling technology. BioCellection's aim is to protect our environment by creating innovative recycling processes for currently hard-to-recycle post-consumer waste plastics by converting waste into quality building blocks for sustainable supply chains. Our innovations unlock the potential of using plastic waste to replace fossil fuel as a resource for creating new materials.

### **Darren Post**

### **NOVA** Chemicals

Darren Post is currently Business Development Manager in NOVA Chemicals ARCEL division. He has been doing Business Development work for ARCEL for the past 16 years, with the previously 10 years on the West Coast as EPS/ARCEL Sales Representative proceeded by 2 years selling to the automotive industry. His first 6 years in the industry were in Urethane Technical Service for Texaco and then ARCO Chemical.

### **Ben Scott**

### GreenMantra Technologies

Ben is the Director of Technology at GreenMantra Technologies. During his time at GreenMantra, Ben has worked on a number of cutting-edge research projects.Ben was part of the core research team that developed a novel

process to take waste polystyrene and convert it into specialty polymers and is currently focussed on improving and expanding GreenMantra's technology and application space. Ben has developed several trade secrets while at GreenMantra and is also the lead inventor on multiple patents. In addition, in 2018, Ben received the Young Leader Award from Canadian Plastics Industry Association.

### Waste Valorization (plastics and more)

### **Craig Gorin**

### Dow Chemical

Craig Gorin is an Associate Research Scientist in Core R&D at Dow, working on materials development in a diverse array of application areas. Currently, he is leading a set of technical efforts to enable improved polymer recycling. Craig's earlier work led to the commercialization of award winning, novel 3D-printing materials (R&D 100 Awards, Edison Award). Prior to joining Dow in 2014, he obtained an undergraduate degree in Chemistry at Harvard University, and a PhD in Chemistry at Stanford University. His thesis work focused on using electrostatics to influence catalytic selectivity.

### Lucas D. Ellis

### National Renewable Energy Laboratory

Lucas D. Ellis received his B.S. from California Polytechnic State University, M.S. from Dartmouth College, and Ph.D. focusing on heterogeneous catalysis from the University of Colorado. He is currently a Director's Postdoctoral Fellow at the National Renewable Energy Laboratory (NREL). His research focuses on developing heterogeneous catalysts and chemical processes capable of enhancing our societies environmental sustainability. This focus on sustainability has been true early in his career as a Research Technician pursuing lignin valorization technologies, to his stint working at a cellulosic ethanol start-up, pursuing cost-effective lignocellulosic pretreatment processes, and now as a Director's Postdoctoral Fellow at NREL, developing novel plastic upcycling technologies to monetizing recycling efforts. He has authored 13 peer-reviewed publications and 2 patents.

### **Scott Nicholson**

### National Renewable Energy Laboratory

Scott Nicholson joined the staff of the National Renewable Energy Laboratory in 2016. He has been involved in a variety of projects focusing on environmental impact and life cycle assessment modeling, as well as electricity capacity expansion modeling. Scott's research has recently focused on the plastics sector, comparing petrochemical-derived plastic supply chains to those of novel, bio-derived polymers. Scott holds a Bachelor's degree in chemical engineering from Tufts University and a Master's degree in Mineral and Energy Economics from the Colorado School of Mines.

### Sustainable Process Design and Manufacturing

### Paul Yelvington

### RAPID Manufacturing Institute

Paul Yelvington is the Chief Technology Officer of the RAPID Manufacturing Institute. Prior to this role, Paul served as the Chief Chemical Engineer and Group Leader for Energy Conversion Technologies at Mainstream Engineering (MEC), where he led programs to develop several modular process technologies, including a portable fast-pyrolysis process for thermochemical biomass conversion to fuels, a hybrid hydrothermal liquefaction process for conversion of wet food wastes to fuels, and a biogas-tolerant engine-generator for agricultural waste digesters. In addition, Paul coordinated MEC's other energy conversion programs and managed the chemical engineering staff. Prior to joining MEC, Paul worked at Aerodyne Research where he studied the emissions of trace gases and volatile particles from aircraft engines, helping to better understand the impacts of aviation on local air quality and climate change.

Paul's expertise includes combustion, alternative fuels, engines, biomass conversion, applied spectroscopy, reactor piloting, techno-economic analysis, technology transfer, product development, and project management. He also specializes in the use of advanced simulations and controls to improve the efficiency of practical energy conversion

devices. Over the years, he has directed over 20 research, development, and engineering programs for industry and government clients at DOD, DOE, NIH, and the USDA.

### Sustainable Social-Ecological Systems

### **Ben McCall**

### Hanley Sustainability Institute

Ben McCall serves as the Executive Director of the Hanley Sustainability Institute at the University of Dayton, where he is also a Professor of Physics and Chemistry. In addition to advancing sustainability education, research, and community engagement, Ben advocates for enterprise-wide changes to make the university's operations sustainable and carbon-free. Prior to moving to the University of Dayton, Ben was a Professor of Chemistry, Physics, and Astronomy at the University of Illinois at Urbana-Champaign, where he led a research group studying molecular spectroscopy and astrochemistry. He is a fellow of the American Physical Society and The Optical Society (OSA).

### Michael Ben-Eli

### The Sustainability Laboratory

Michael Ben-Eli is the founder of The Sustainability Laboratory, established in order to develop and demonstrate groundbreaking approaches to sustainability practices, expanding prospects and producing positive, life affirming impacts on people and ecosystems in all parts of the world.

Prior to launching The Lab, Michael pioneered applications of Systems Thinking and Cybernetics in management and organization. Over the years he worked on synthesizing strategy issues in many parts of the world and in diverse institutional settings, ranging from small high technology firms to multinational enterprises, manufacturing companies, financial institutions, health care and educational organizations, government agencies, NGOs, and international multilateral organizations including the World Bank, the United Nations Environment Program, the Global Environment Facility, and others.

### Innovation for Sustainable Businesses and Industries

### **Mark Miller**

### **Biosynthetic Technologies**

Mark Miller is the CEO of Biosynthetic Technologies (BT), an Indianapolis-based company that provides high performance, renewable, non-toxic, biodegradable base fluids. Mr. Miller is a serial entrepreneur with a special emphasis on bio and sustainable technologies. Prior to BT, he co-founded and was CEO of Terresolve Technologies, Ltd. an environmentally safe chemical products company. He led the Organization from start-up until his exit, creating a multimillion dollar, highly profitable, global industry leader. He has engineered, sold and marketed environmentally acceptable lubricants and base oils for over 30 years.Mr. Miller has a B.S. in Chemical Engineering from Tufts University and an M.B.A. from Manhattan College. He also sits on the Board for The National Foundation For Animal Rescue (NAFFAR) and he and his wife, Shari, have adopted more than their share of homeless critters.

### Decarbonization

### **Alexandros N.Karaiskakis**

### **Bioenergy Devco**

Alexandros Karaiskakis is the Director and Head of Science, Technology, and Business Innovation department in Bioenergy Devco, a global leader in designing, operating, building, and financing anaerobic digestors company. In his current role, Dr. Karaiskakis ensures that Bioenergy DevCo is at the forefront of scientific and business innovation through innovative approaches, technologies, and partnerships that are aligned with sustainability and circular economy principles.

Alexandros has more than 15 years of experience in Sustainable Energy Systems, Green Chemistry, Data Analytics, and Sustainability projects in both academia and industry. His scientific research was focused on CO2 conversion to green fuels and chemicals and the conversion of organic compounds to biofuel. Alexandros also worked in various

technology assessment projects, including Life Cycle Assessment methodology for industrial, academic, and public policy purposes. He also founded ReInDev, an initiative to reinvent industrial and corporate growth through Science, Innovation, Sustainability, and Data Analytics.

### **Elizabeth Nesbitt**

### U.S. International Trade Commission (USITC)

Elizabeth R. Nesbitt, a Senior International Trade Analyst at the U.S. International Trade Commission (USITC), follows trade and competitiveness issues related to pharmaceuticals, biotechnology, and nanotechnology. She has been a project leader and/or major author on a wide variety of USITC reports, addressing topics ranging from industrial biotechnology to SMEs to prescription drug pricing, as well as the author of articles on bioproducts, the circular economy, and pharmaceuticals. She has made multiple presentations as an invited speaker, addressing these topics and others.

Ms. Nesbitt's numerous professional awards include the USITC's Distinguished Service Award in 2012 and, from the Association of Women in International Trade (WIIT), Outstanding WIIT Member of the Year in 2004 and the WIIT Lifetime Achievement Award in 2013. She earned a B.S. in chemistry and an M.S. in chemical engineering from Manhattan College. She is active (including as a Board member) in several organizations, particularly those promoting STEM education.

### **Kylee Harris**

### National Renewable Energy Laboratory

Kylee Harris is a process research engineer at the National Renewable Energy Laboratory in Golden, Colorado. Her work in the Techno-Economic, Sustainability, and Market Analysis group centers around techno-economic analysis (TEA) and life cycle assessment (LCA) for biomass conversion technologies. Prior to joining NREL in 2019, Harris received her B.S. in Chemical and Biological Engineering at Colorado State University where she participated in biocompatible polymer research and competed in AIChE's annual student Chem-E Car competitions.

### **Ravi Malhotra**

### ICAST

Ravi has 31 years of experience as a social entrepreneur and engineer. He has led award-winning R&D efforts and has successfully launched eight new social ventures. Ravi's focus is on driving market-based sustainability via green retrofits, consulting, and investment for smarter multifamily housing through two nonprofit ventures: Triple Bottom Line Foundation (www.tblfund.org) – a CDFI that provides green energy financing, and ICAST (www.icastusa.org), which provides clean energy design, development, planning and construction services.

### Renewable/Alternative Energy

### Silvia Palma-Rojas

### California Energy Commission

Dr. Palma-Rojas is a program manager at the California Energy Commission's Research Division, leading the research wind and solar energy portfolios. She also supports the research program of renewable energy forecasting, bioenergy, and small hydropower. Before the Energy Commission, Dr. Palma-Rojas worked as an economist consultant in international organizations, life cycle assessment adviser for the Federal Government of Brazil, and researcher in the Departments of Economics and Engineering of the University of Brasilia, Brazil. Dr. Palma-Rojas holds a PhD in Economics and a master's degree in Mechanical Engineering, with +17 years of experience in the research areas of energy economics, sustainability, life cycle assessment, and renewable energy and biofuels.

### Shudipto K. Dishari

### University of Nebraska-Lincoln

Dr. Shudipto Konika Dishari is an assistant professor at the Department of Chemical and Biomolecular Engineering at University of Nebraska-Lincoln (UNL) (2016- present). She was a post-doctoral fellow in Chemical Engineering (PI: Andrew Zydney), and Materials Science and Engineering (PI: Michael Hickner) at the Pennsylvania State

University. Dishari graduated from the National University of Singapore with a Ph. D. in Chemical and Biomolecular Engineering. Dishari's research focuses on designing synthetic, bio-derived, and nature-inspired ion-conducting and light-harvesting polymers. Dishari explores the fascinating interfacial and nanoscale phenomena within polymeric confined systems. Her work targets to impact energy conversion/storage devices, chemobiosensing, and biomedical applications. Dishari has received several honors and awards in recognition of her innovative research, extraordinary teaching abilities, and academic promise, including: Department of Energy (DOE) Office of Science Early CAREER Award (2019-2024), National Science Foundation (NSF) CAREER Award (2018-2023), EPSCoR First Award (2017-2018), Nebraska Center for Energy Science Research Award (2020-2021), Baxter Young Investigator Award (2014), Henry Y. Kleinkauf Family Distinguished New Faculty Teaching Award (2020), and Harold and Esther Edgerton Junior Faculty Award (2019).

### Wade Braunecker

### National Renewable Energy Laboratory

Dr. Braunecker is a Senior Scientist at the National Renewable Energy Laboratory. He earned his bachelor's degree in chemistry from the University of Notre Dame and his doctorate in polymer chemistry at Carnegie Mellon University in Pittsburgh, Pennsylvania. Dr. Braunecker has nearly two decades of experience in synthesis of advanced functional polymers. As Principal Investigator of the organic photovoltaic (OPV) thrust in the Solar Energy Research Institute of India and the United States (SERIIUS), he coordinated research between synthesis, characterization, and device groups among various U.S. and Indian institutions, focusing on the development of fluorinated OPV materials with enhanced photostability. Dr. Braunecker has also worked on a number of projects for battery applications, including the design and synthesis of polymers with pendent nitroxide radical groups for application as organic radical cathode materials, the development of materials for hybrid flow batteries, and workfunction tuning of solid-state electrodes. More recently, he has been developing covalent organic frameworks for gas storage and separation applications under EERE/FCTO's Hydrogen Materials—Advanced Research Consortium (HyMARC).

### Nutrient Pollution, Prevention, and Control

### Anne W. Rea

### U.S. Environmental Protection Agency

Anne W. Rea is a Senior Science Advisor in the Center for Public Health and Environmental Assessment within the U.S. Environmental Protection Agency's Office of Research and Development. Prior to this she was the Associate National Program Director for Nutrients and Harmful Algal Blooms in the US EPA's Safe and Sustainable Water Resources Research Program. She leads the integration of cross-cutting research related to nitrogen and associated co-pollutants within the US EPA and with other federal, state, and NGO partners. Dr. Rea also coordinated and managed contributions to US EPA's former Ecosystem Services Research Program. For several years she was a team lead and risk assessor in US EPA's Office of Air Quality Planning and Standards for both air toxics and the secondary National Ambient Air Quality Standards. She also coordinated and led the Office of Air's ecological risk program for air toxics and Ecological Research Coordination Team.

### Gerardo J. Ruiz-Mercado

### US Environmental Protection Agency

Gerardo J. Ruiz-Mercado is a senior research manager designing sustainable processes, developing methods and tools for nutrient and waste management, supply chains, life cycle inventory and assessment, and bioenergy systems, process design, modeling, and optimization. He is currently leading and developing U.S. Environmental Protection Agency research projects on decision support methods and tools on evaluating techniques, economics, logistics for the repurposing of primary sources of nutrient pollution and chemical waste, and subsequent ecosystem and human health impacts. Such tools would help to reduce energy/material consumption and environmental impacts and increase the profitability of chemical and energy systems. He is an expert in sustainability evaluation, process system engineering, supply chain design, organic waste management, nutrient pollution, and life cycle approaches. He has over 40 peer-reviewed publications, organized technical conferences, and sits on the editorial board of the Processes journal and the Clean Technologies and Environmental Policy

journal. Also, the manager of the diversity and inclusion EPA Hispanic employment program. Gerardo has volunteered his time to the AIChE, serving as the programming Chair of the Environmental Division, session Chair, and International Advisor of the Sustainable Engineering Forum. In 2019 he chaired the Enterprise and Infrastructure Resilience Conference.

### Mikaela Algren

### Colorado School of Mines

Mikaela Algren just finished her third year as a graduate research assistant in the Civil and Environmental Engineering Department at Colorado School of Mines. She studies nutrient use and management, with a primary focus on nitrogen and phosphorus in the production of agricultural commodities in the United States. She enjoys reading, cooking, and being active outdoors through running, cycling, and swimming.

### Food, Energy, Water Nexus

### Brian Kolodji

### Black Swan, LLC

The founder of Black Swan, LLC, an Intellectual Property Rights Holding Company, and Kolodji Corp, for Energy Carbon Management, Mr. Kolodji for the past over 40 years has been blessed in helping promote and fully implementing chemical engineering solutions for the most challenging chemical engineering issues; from resolving acid rain with the Parsons Corporation, to post-Bhopal process safety and risk management solutions with Union Carbide and India, to post-BP Macondo/Deep Water Horizon solutions offshore with UOP/MODEC/Petrobras/BP. Mr. Kolodji, as presenter at 2018/19/20 and chair of the 2019/20 AIChE Spring National Meeting's Carbon Management and Sustainability sessions, has been hailed by industry, and fellow presenters presenting their work from USDA and Brookhaven National Laboratory for his trademark Black Swan Cycle. Mr. Kolodji, is setting his sights on resolving the energy/water/food nexus riddle by fully implementing greenhouse gas reduction solutions to reverse global warming by 2030 with the Black Swan Cycle of energy carbon management technologies.

### Daniela Gormaz

### University of Chile

Daniela Gormaz is a student of Chemical Engineering at the University of Chile, where she has also been a teaching assistant for the last three years. Daniela completed a three months internship with the Toulouse INP- ENSIACET in France. Now, she is in charge of a FONDECYT project about optimization in water networks. Her interests include the design and development of sustainable solutions, and she is eager to participate in the academy world.

### **Short Presentations**

### Alin Semenescu

### West University of Timisoara

Alin Semenescu is a Ph.D. researcher at the West University of Timisoara. After graduating with a BSc in Psychology and a MSc in Social Psychology from Groningen University, he returned to the West University of Timisoara to continue his research on urban mobility. His research focuses on the psychological determinants of different mobility styles and on the efficiency of psychological interventions in motivating urban residents to choose sustainable means of transportation instead of the car.

### Farah Ramadan

### Texas A&M University

Farah Ramadan is a chemical engineering student at Texas A&M University at Qatar with an interest in process integration and optimization for sustainable design. She is currently a rising senior and plans to continue her studies and peruse a Master of Science degree in chemical engineering.

### **Elizabeth Abraham**

Elizabeth Abraham is a chemical engineer who is passionate about sustainable development and plans to pursue a Masters's program in process systems engineering to help develop sustainable systems for tomorrow.

### Taha Kubbar

### TAMUQ

Taha Kubbar is a Chemical Engineer who is passionate about the environment and sustainability. He obtained his BSc from Texas A&M University at Qatar class in 2020 and plans to pursue an MSc degree in Chemical Engineering from TAMUQ starting fall of 2020.

### **Kim Tutin**

### Georgia-Pacific Chemicals LLC

Education: Bachelor's degree in Chemistry from the University of Minnesota, Morris and an MBA in Technology & Engineering Management with a 3.91 GPA from City University of Seattle. Technical commercialization experience includes identification, screening, development, scale up, & commercialization of new technologies for private sector industry including emissions control equipment and new resin adhesives. Project Management experience includes successful development and scale up of a pilot unit to control emissions from wood drying using Bead Activated Carbon (BAC) in a Fluidized Bed Concentrator (FBC). Effort included technology identification, testing, intellectual property creation, collaboration with partner company Environmental C&C, coordination with multiple intracompany divisions and across multiple functional capabilities, internal and external sales.

### Pranjal Maheshwari

### Rajiv Gandhi Institute of Petroleum Technology

Pranjal is a Chemical Engineering Sophomore at Rajiv Gandhi Institute of Petroleum Technology, India ready to fuel the future. He is a gold medalist with a consistent academic record. His research aims to create alternatives that could fulfill the decreasing pool of global energy resources as it is becoming increasingly essential to optimize the processes central to modern life involving; CO2 Capture through Modeling, Simulation, and Experimental approaches using different types of sorbents and wishes to contribute to the broader scientific community by creating new paradigms in engineering and research.

### **Ramsharan Pandey**

### North Dakota State University

Ramsharan Pandey is a PhD student in the Department of Coatings and Polymeric Materials at North Dakota State University. His current work focuses on the economic and environmental assessment of lignin-based polymers. His research interests include sustainability assessment of biobased materials, biomass conversion to fuels and chemicals, and life cycle optimization of biobased materials production. Ramsharan has a bachelor's degree in Mechanical Engineering and a master's degree in Agricultural and Biosystems Engineering.

### Rehana Ali

### University of Trinidad and Tobago

Rehana Ali holds a Bachelors (B.Sc.) Degree in Chemical Engineering and Masters of Science (M.Sc.) degree in the field of Project Management. After a successful career in industry, Rehana joined academia in 2016 and currently holds the position of Senior Instructor in the Process Engineering Programme at the University of Trinidad and Tobago, where she lectures a variety of courses such as Unit Operations Lab, Utilities and Systems, Process Upsets and Troubleshooting and Equipment Maintenance presently. She has researched the areas of material science and rheology. She is currently pursuing a Masters of Philosophy (M.Phil.) degree at the University of Trinidad and Tobago, focusing on the reduction of greenhouse gases (GHG) in Trinidad and Tobago.

### Safiyyah Wahid

### University of Trinidad and Tobago

Safiyyah Wahid holds a Bachelors (B.Sc.) Degree in Chemical Engineering from the University of the West Indies, Trinidad & Tobago. She also holds Diplomas in Project Management and Safety Management, Policies and Procedures. After a successful career in industry as an Operations Supervisor, Ms. Wahid joined academia in 2013 and currently holds the position of Instructor II in the Process Engineering Programme at the University of Trinidad and Tobago where she currently lectures in Mass Transfer & Separation processes, Industrial Processes and Process Safety based courses, oversees the Co-Op internship students and supervises Chemical Engineering Design Project students at the Diploma level. Ms. Wahid is currently pursuing an MPhil Degree in the area of Waste Management Strategies for Sustainable Development in Trinidad & Tobago.

### Sharona Mohammed

### University of Trinidad and Tobago

Ms. Sharona Mohammed is a Research Assistant under the Process Engineering Department at the University of Trinidad and Tobago. Having graduated with her Bachelor of Applied Science Degree in Process Engineering from the University of Trinidad and Tobago, she is currently pursuing her Masters of Philosophy in the area of optimizing natural resource production. Her field of study is focused on investigating the impact of asphaltenes precipitation and deposition in the upstream and downstream sections of the oil industry in Trinidad and Tobago. In conjunction with this, Ms. Mohammed is actively involved in research in the field of sustainable waste material utilization to promoting economic generation whilst adhering to environmentally sound practices. Employing recycling and reuse technologies to enhance infrastructural development, the research is hinged on assessing the impact on the rheological properties of asphaltic materials as a result of waste material incorporation.

### Zahra Karimi

Auburn UniversityZahra received her B.S. degree in Chemical Engineering from Sharif University of Technology in Tehran, Iran, in 2016. She is currently pursuing a Ph.D. degree in Chemical Engineering in Auburn University under the supervision of Dr. Virginia Davis and Dr. David M. Blersch. Her research interests include attached algal cultivation systems, algae cell-surface interactions, surface thermodynamics, polymer composites, additive manufacturing.

### Muhammad Ajaz Ahmed

### Seoul National University

Dr. Ahemd Muhammad Ajaz earned his Ph.D. degree from the Korea Advanced Institute of Science and Technology (KAIST) in 2017. He is an Authoraid official mentor and has published more than 25 peer-reviewed articles, three book chapters, and 15 conference papers. Recently, he has been working at the Seoul National University in South Korea as a Korea Research Foundation (KRF) postdoc fellow. He is passionate about developing new strategies to use biorefinery waste (lignin) to be used as refined resource products with interests to incorporate proto lignin as well as plastics for the production of sustainable fuels and materials.

### **ZOOM GUIDELINES**

### Preparations before the Virtual Conference

### Prepare your Voice

Troubleshoot your microphone—do a recording test with both video and audio and see if you are satisfied with the quality. If the microphone on your computer is not working to the best of its ability, consider obtaining an external microphone to sound clearer during your presentation.

### Prepare your Space

Adapt the room you will use so it suits your speech and make sure there are no elements in there that might shift the focus of your audience—clean everything around you and hide anything that may seem out of place. Zoom Backgrounds are a great way to cover your surroundings, so you stay in focus throughout your entire presentation.

Make sure there is an adequate amount of light on you, the subject, during your talk. Make sure there are no light interferences/shadows that can ruin your presentation. One good tip is to face your light source rather than having it behind you.

A poor internet connection can be detrimental to your presentation; make sure to test your Wi-Fi before the online event. If possible, and to make sure you will not encounter any issues, try using a cable connection instead.

### Practice before going Live

Before going on live for the first time, test your gear (your microphone, camera, and lighting), your presentation and let your family & friends know when you will be presenting so you have no interferences.

Practice your entire presentation before your talk, so you know how you will sound, what you look like, and what is comfortable for you!

### CODE OF CONDUCT

### CODE OF CONDUCT

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.
- 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 Chem-E-Car Competition<sup>®</sup>, should also comply with all applicable safety guidelines.

Any violations of the foregoing should be reported to the President or the Executive Director of the Institute.



ICOSSE 20 International Congress on Sustainability Science & Engineering

## **ABSTRACT BOOK**



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### Monday, August 3rd, 2020

### **KEYNOTE**

#### LEVERAGING SUSTAINABILITY REGARDING PLASTIC: LAW AND POLICY LANDSCAPE

### Mary Ellen Ternes

Earth & Water Law, LLC, Oklahoma City, OK

Environmental law and policy are designed to mitigate the harmful effects of pollution. Yet, plastic generally tends to fall outside the scope of stringent environmental regulation, depriving entities producing or distributing plastic from specific critical incentives that could best support their development of meaningful, sustainable approaches. Familiar approaches to designing environmental law and policy are not specifically designed to address persistent synthetic materials such as the current suite of commercial synthetic plastics distributed in the market today. Environmental programs generally focus on addressing pollution by mitigating exposure to chemicals that pose a threat of acute and chronic toxicity, including carcinogenicity. The synthetic macro and microplastics in our environment, while likely leaching some chemical pollutants have observably caused harm through their persistence in the environment resulting from their inert nature. Through their characteristics of fracturing into smaller and smaller particles while not dissolving, reacting, or degrading, synthetic plastics may result in significant acute and chronic harm from physical obstruction of biological processes, whether as macro, micro or nanoparticles. This harm is generally not mitigated through conventional environmental regulation focusing on mitigating chemical toxicity. Ongoing research that better defines this harm, and provides reproducible parameters, metrics, and nomenclature for such harm, will support the development of new approaches to mitigating such harm. These new approaches can support the better application of existing law and policy while also informing the development of more tailored authority to address this type of environmental pollutant. These new approaches also support litigation and other methods of distributing the burden of risk and harm better defined from this research once the harm can be quantified. This presentation will summarize the current status of global policy approaches, including the United States, and how both ongoing efforts to qualify and quantify harm, and these new legal and policy measures, serve to provide a significant incentive for all plastic dependent industry sectors to seek more meaningful approaches to sustainability, with the critical goal of keeping plastic out of the environment.

### SUSTAINABLE SUPPLY CHAINS (LOGISTICS MANAGEMENT)

### THE EFFECT OF GROWER CHARACTERISTICS AND FARMING DECISIONS ON SUPPLY CHAIN ESTABLISHMENT FOR BIOFUELS.

### **Damon Hartley**<sup>1</sup>, Pralhad Burli<sup>1</sup>, and L. Michael Griffel<sup>2</sup>

(1) Idaho National Laboratory, Idaho Falls, ID, (2)Bioenergy Analysis, Idaho National Laboratory, Idaho Falls, ID

Biorefinery supply chain establishment and operation costs have been one of the barriers to a successful bioenergy industry. The commercial development of biofuels and bioproducts depends on whether renewable biomass feedstock is available while not directly competing with the production of food. Farmers are one of the most important stakeholders in the biofuel supply chain, and increasing farmer participation is necessary for the eventual success of the bioenergy industry. Meanwhile, grower risk perception, the structure of the bioenergy supply chain, market demand, alternate uses for their feedstock, and risk mitigation could have important ramifications for grower participation. We developed an agent-based modeling framework to simulate farmer bioenergy crop adoption behavior across a 50-county study region in Nebraska, Kansas, and Colorado. The purpose of the framework is to model a system where the behavior of the agent is not known with complete certainty, but rather dictated by probability or random events. We studied grower participation levels for supplying corn stover and converting land into perennial energy crop production and examine the influence of farm attributes, market structure, social networks, media influence, and individual characteristics on farmer decisions. We found that the acreage of adopted perennial crops was considerably less than the total acres with residue removal. The model helps assess the propagation of individual-level decisions on bioenergy feedstock supply for a specific region. Furthermore, identifying levers that have the most impact on grower adoption has important implications for the future of the industry.

### PROJECTIONS FOR ENERGY USE, COSTS, AND EMISSIONS FROM RECOVERY OF CRITICAL MINERALS FROM NIMH BATTERY RECYCLING IN THE U.S.

### *Chukwunwike Iloeje*<sup>1</sup>, Alinson Santos Xavier<sup>1</sup>, **Sarang Supekar**<sup>1</sup>, and Diane J. Graziano<sup>2</sup> (1)Energy Systems, Argonne National Laboratory, Lemont, IL, (2)Argonne National Laboratory, Lemont, IL

This paper develops prospective estimates of life cycle energy use, costs, and emissions associated with a large-scale Nickel-metal hydride (NiMH) vehicle battery recycling infrastructure to recover critical minerals. NiMH batteries contain substantial quantities of Nickel (Ni), Cobalt (Co), and rare earth elements including Neodymium (Nd) and Praseodymium (Pr), all of which are deemed critical to a clean energy and transportation future in the U.S. As of hybrid and mild-hybrid vehicles containing NiMH batteries near their end-of-life (EOL) in the coming decades, systematic recovery of these minerals can offset the country's reliance on foreign imports, thus contributing to securing their long-term supply in a circular economy. In this work, we develop an optimization model, based on Mixed-Integer Linear Programming (MILP), to determine the most cost-effective location and sizing of recycling facilities, based on inputs from a stock-and-flow model of NiMH vehicle batteries. Material flows developed from this model integrate with a physical separation and Gibbs Energy minimization-based solvent extraction process simulation that model key components of the recycling logistics pipeline. The optimization model outputs include annual mass flow rates of recovered Ni, Co, Ce, La, Nd, and Pr from EOL NiMH batteries, to which the overall energy use, costs, and emissions are ascribed using an economic allocation method. Uncertainties in geographic distribution EOL batteries, collection and transportation of EOL batteries, critical material recovery, and extraction process, and energy sources along the recovery value chain are also considered. Energy use and costs of recovered critical materials along with their key drivers are compared with corresponding energy and cost values for the materials from virgin sources.

### IMPACTS OF ENVIRONMENTAL POLICY ON SUPPLY CHAINS.

**Philip Tominac** and Victor M. Zavala Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

Supply chains are complex networks of economic activities comprising interacting stakeholders, global markets, and multiple incentives [1,2]. Supply chains are also associated with the production of various factors that negatively impact air and water quality. Policymakers seek to incentivize sustainable, low impact supply chain practices. Typically, sustainability and economic incentives conflict. We have recently shown that conflicting incentives can be systematically analyzed by using a coordinated market interpretation of supply chains [3]. Coordinated markets have useful economic properties related to inherent product values (pricing) and stakeholder remuneration. This interpretation is useful in policymaking, where the objective is to incentivize sustainable practices without destroying economic incentives.

We use a theoretical analysis of supply chain formulations to characterize market incentives and outcomes under the environmental policy. In the proposed framework, we include the policymaker as a market stakeholder that bids against environmental emissions and thus becomes an economic driver in the market. Our approach allows us to determine the economic value of the environmental policy and the extent to which policy results in a market collapse. Moreover, we are able to characterize supply chain production regimes in terms of environmental policy implementations. This framework provides an approach to determine a policy that achieves sustainability objectives while maintaining economic incentives in markets. We apply this methodology to organic waste management infrastructure in the city of Milwaukee, WI. The city has defined a landfill management objective of 40% organic waste diversion [4]. We demonstrate that policy implementations (environmental taxes) can achieve this solution, and propose alternatives based on market insights.

### COMPETITION OF RENEWABLE FEEDSTOCKS

### A FRAMEWORK FOR ASSESSING THE SOCIAL SUSTAINABILITY OF GUAR AGRICULTURE.

### VeeAnder Mealing<sup>1</sup> and Amy E. Landis<sup>2</sup>

(1)Civil & Environmental Engineering Department, Colorado School of Mines, Golden, CO, (2)Civil and Environmental Engineering, Colorado School of Mines, Golden, CO

With continued drought predictions for the southwest, it is important to explore drought-tolerant crop adoption options that have the potential to produce high-value products, minimize risk and impacts, and maximize product development profit. Guar (Cyamopsis tetragonoloba) is an annual desert legume; its gum is used as an emulsifier in the food industry and in the oil and gas industry during the recovery process. The rise of hydraulic fracturing for shale oil production has significantly increased the world market demand for processed guar and resulted in unmet domestic demand for guar products and co-products in the US. As we begin to cultivate a new industrial crop in the US, there are significant opportunities to enhance the sustainability, yield of guar gum, and support its economic advantages for Southwest US. Thus, in order to guide the growth of guar and its products down a sustainable path, we must quantitatively assess the environmental, economic, and social impacts for the production of guar gum and its co-products. Holistic sustainability assessment methods that address all three pillars of sustainability are rare. While there are studies focused on assessing the environmental and economic sustainability of guar agriculture, our study will focus on the social sustainability and potential ways of integrating the social impacts with the existing economic and environmental studies. The goal is to develop a framework for assessing the social pillar of guar cultivation in the southwestern United States while addressing the unique challenges that come with emerging technologies like the emerging feedstock of guar in the US. The social sustainability tools that will be used in this study are Social-Life Cycle Analysis, Social impact assessment, and site-specific interviews. The unique collaboration of researchers and industry in the USDA Sustainable Bioeconomy for Arid Regions (SBAR) project allows us the opportunity to collect social sustainability data from experts and evaluate their potential to integrate into environmental and economical methods.

### **BIO-RESTORE: BIOMASS TO RESTORE NATURAL RESOURCES**

### MULTI-CRITERIA LAND SUITABILITY ANALYSIS: IDENTIFYING AREAS TO DEPLOY INTEGRATED LANDSCAPE MANAGEMENT FOR BIOENERGY FEEDSTOCK PRODUCTION.

### *L. Michael Griffel*<sup>1</sup>, Yingqian Lin<sup>2</sup>, and Damon Hartley<sup>2</sup>

(1)Bioenergy Analysis, Idaho National Laboratory, Idaho Falls, ID, (2)Idaho National Laboratory, Idaho Falls, ID

Converting low-yielding subfields within agricultural production fields to energy crop production has been demonstrated to improve field profitability, biomass availability, soil carbon sequestration, and mitigate soil erosion. Integrated Landscape Management (ILM) is a strategy developed to integrate biomass production into agricultural production fields to reduce feedstock access costs while improving the sustainability of crop production systems. The goal of this study is to develop a multi-criteria land suitability analysis to identify fields in which an ILM strategy will likely result in maximized economic and environmental benefits. Evaluation criteria were developed across three domains: agronomic, field operability, and environmental. The set of criterions were used to develop a linear fuzzy-logic prediction model, which was used to calculate the site suitability index for each field. To demonstrate the ILM site suitability criteria method, this analysis was applied to Smith County in north central Kansas, which is included with the larger study area that has been identified and used for feedstock logistics modelling in support of the annual Bioenergy Technologies Office (BETO) State of Technology reports on herbaceous biomass supply systems. Data were compiled for this county which consisted of 19,614 individual parcels defined by United States Department of Agriculture common land unit data. Analysis results showed that the ILM site suitability model identified and scored 5,527 parcels as potentially suitable for ILM.

### **BIOMASS CONVERSION TECHNOLOGIES**

### PREPROCESSING REACTOR-READY FEEDSTOCKS FOR THERMOCHEMICAL CONVERSION.

**David Lanning**<sup>1</sup>, Jim Dooley<sup>1</sup>, Christopher Lanning<sup>1</sup>, Neal Yancey<sup>2</sup>, and Damon S. Hartley<sup>3</sup> (1)Forest Concepts, Auburn, WA, (2)Idaho National Laboratory, Idaho Falls, ID, (3)Bioenergy Analysis, Idaho National Laboratory, Idaho Falls, ID

Developing cost-effective methods for processing biomass into an economic biofuel product is critical to the success for the bioenergy industry in the United States. Size reduction and drying of the material, where used, are two of the most costly and energy-intensive operations that are undertaken during preprocessing. Reducing the energy required during these two phases will lower the cost of processing and ultimately reduce the overall cost to the final user. Forest Concepts developed a paradigm-changing rotary shear comminution technology that enables efficient milling of high moisture and green biomass all the way to final millimeter-scale particle size BEFORE drying when drying is needed and WITHOUT drying when high moisture feedstocks are desired. The rotary shearing technology enables a new energy efficient pathway for pre-processing that includes low-emissions, low-temperature drying in highly efficient moving bed dryers. Rotary shear processed particles have a high surface-area-to-volume and high bulk porosity that enables use of low-temperature (120C), low emissions dryers. Also, by drying after milling, the time from wet to dry is reduced from about 20 minutes for wood chips to less than 5 minutes for rotary-sheared conversion-ready feedstocks. The rotary shear equipment is increasingly considered as an alternative to conventional pathways for pre-processing wood chips and debaled herbaceous biomass into feedstocks for conversion to biofuels, biochemicals, and bioproducts. A 7 ton per hour system was installed at Proton Power, Inc to produce feedstocks for conversion to renewable diesel. Idaho National Laboratory performed a Techno-economic Analysis (TEA) comparing the traditional pathway with a rotary shear followed by drying for 6mm conversion-ready feedstock woody particles. The INL TEA reported that the rotary shear pathway consumed approximately 50% of the drying energy as the conventional hammer mill pathway and may save as much as \$50 million per year in preprocessing costs at a full-scale 800,000 tpy biorefinery. In addition to the rotary shear, Forest Concepts is developing advanced drying techniques that utilizes modular zones to match dryer characteristics to a given material's drying curve. This novel approach will potentially yield an additional 30% energy savings in preparingreactor ready feedstocks.

**MULTIFUNCTIONAL CATALYST DESIGN FOR ONE-POT CONVERSION OF WOODY BIOMASS TO BIOFUEL. Hannah Nguyen**<sup>1</sup>, Daniela Stück<sup>1</sup>, Nabila Huq<sup>2</sup>, Stephen Tifft<sup>2</sup>, Davis Conklin<sup>2</sup>, and Derek Vardon<sup>2</sup> (1)National Renewable Energy Laboratory, Golden, CO, (2)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO

One-pot solvolytic/catalytic conversion of cellulosics to liquid oxygenates in supercritical methanol is an emerging technology in biomass-to-biofuel research field. The process utilizes the same solvent with the reductive catalytic fractionation of lignin and provides potential for a fully integrated biorefinery scheme. Under supercritical methanol solvent and porous CuMgAl mixed oxide catalyst, up to 70% yield to fuel-grade aliphatic alcohols from woody cellulosic residues has been reported. Though promising, the process is still at the proof of concept stage with limited insights into catalyst reactivity, continuous process feasibility, and fuel application of the liquid product. Herein, we proposed a catalyst design strategy of Cu-based mixed oxide for enhanced performance in C2-C6 aliphatic alcohol productions from biomass. Systematic and hypothesis-driven catalyst screening was conducted and benchmarked against the state-of-the-art catalytic material. The reducibility of the support oxide was proposed to be the key catalyst design parameter. The down-selected catalyst was found to increase C2-C6 aliphatic alcohol yield by two-fold compared to CuMgAlOx at the same reaction conditions. A semi-continuous solvolysis/catalysis reactor system was commissioned to investigate catalyst performance in flow reaction, and the process viability was tested at various gram scales of biomass. Lastly, fuel properties of the aliphatic alcohols were experimentally tested to validate performance as a high-grade gasoline blend stock, based on the fuel properties such as energy density, octane number, boiling point distribution, and freezing point.

#### **REVERSIBLY SOLUBLE BASES FOR ALKALINE OXIDATION OF LIGNIN.**

*Jacob S. Kruger*<sup>1</sup>, David G. Brandner<sup>1</sup>, Camille Amador<sup>1</sup>, Katherine Krouse<sup>2</sup>, Daniel Wilcox<sup>1</sup>, and Gregg T. Beckham<sup>1</sup>

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Production of aromatic aldehydes, such as vanillin, from lignin, has been an intriguing process for decades, but widespread implementation has been inhibited by the high hydroxide:lignin ratios required for significant aldehyde yields. In this work, we explore oxidation of lignin-rich residues isolated from corn stover after deacetylation, mechanical refining, and enzymatic hydrolysis (DMR lignin), using reversibly-soluble bases in place of NaOH. In particular, strontium and barium hydroxides have low solubility at room temperature, but become soluble to more than 2 M at temperatures above 100 °C, thus producing highly alkaline conditions at reaction temperature but facilitating a simple recovery and recycle of the alkali upon cooling. Aromatic monomer yields are comparable for both types of bases at 20-30 wt%, depending on the lignin substrate. Overall, these results suggest a strategy to substantially reduce the cost and life cycle impact of lignin depolymerization by alkaline oxidation.

### ENVIRONMENTAL, ECONOMIC, AND SCALABILITY CONSIDERATION OF SELECTED BIOMASS-DERIVED BLENDSTOCKS FOR MIXING-CONTROLLED COMPRESSION IGNITION (MCCI) ENGINES.

**Andrew Bartling**<sup>1</sup>, **Pahola Thathiana Benavides**<sup>2</sup>, Troy R. Hawkins<sup>2</sup>, Steven D. Phillips<sup>3</sup>, and Avantika Singh<sup>1</sup>

(1)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO, (2)Argonne National Laboratory, Lemont, IL, (3)Pacific Northwest National Laboratory, Richland, WA

Economic and environmental favorability are vital considerations for large-scale development and deployment of sustainable fuels. Under the Co-Optimization of Fuels & Engines (Co-Optima) project, a Department of Energy (DOE)sponsored project, we have conducted economic and sustainability analyses of pathways for producing bioblendstocks optimized for improved combustion for mixing-controlled compression ignition (MCCI) engines. Over the past two years, we assessed 15 pathways including use of a variety of renewable feedstocks and conversion technologies to produce target fuels. We used techno-economic analysis (TEA) and life-cycle analysis (LCA) to determine which bioblendstock candidates are likely to be viable in terms of affordability, sustainability, and state of technology. A slate of 19 metrics evaluating technology readiness, economic viability, and environmental concerns was established with each metric ranked as either favorable, neutral, unfavorable, or unknown for each evaluated pathway. Among the results, we found that the economic metrics were largely favorable for most of the bioblendstocks and further economic improvements could be realized in biochemical pathways when lignin valorization is included. Most of the conversion technologies were determined to be robust in that they would be minimally affected by the feedstock specifications and variations. However, given the early stage of development for most of the pathways, blending behavior and testing for legal limits are key data gaps as knowledge of how many of these bioblendstocks will perform when blended with existing fuels and how much can be added while still meeting legal specifications are still being assessed. Most of the bioblendstocks showed significant reductions in lifecycle greenhouse gas (GHG) emissions and fossil energy consumption relative to conventional diesel fuel, with eight pathways showing the potential for a reduction of greater than 60% for both metrics. Results from these analyses enable researchers and industry assess the potential viability of MCCI bioblendstocks.

### STRUCTURAL AND VALORIZING PROPERTIES OF NATIVE LIGNIN FROM NATURAL VARIANT POPLAR.

**Arthur J. Ragauskas**<sup>1</sup>, Nathan Bryant<sup>2</sup>, Jin Zhang<sup>3</sup>, Chang Geun Yoo<sup>4</sup>, Yunqiao Pu<sup>5</sup>, and Wellington Muchero<sup>6</sup>

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Second generation lignocellulosic biomass crops, such as Populus trichocarpa, are a encouraging renewable alternative to current petroleum based fuels. However, in order to be viable, new bioenergy feedstocks will need to be engineered for sustainable production and efficient conversion to biofuels and bioproducts. This is in part to address the inherent recalcitrance of lignin to enzymatic hydrolysis. By analyzing the structure of native lignin from a GWAS population of Populus trichocarpa, it is possible to utilize phenotype-to-genotype correlations to identify the genetic basis of lignin variation. To support this effort, we have utilized 2D HSQC NMR to analyze over 350 unique genotypes of naturally variant Populus trichocarpa. This analysis has provided insights to the relative abundance and variation of syringyl, guaiacyl, p-hydroxyphenyl, and p-hydroxybenzoate units, as well as aryl ether, phenylcoumaran, and resinol linkages. Gene expression analysis of these results has identified several candidate genes and transcription factors which may impact cell wall biosynthesis. In addition, subsets of lignin samples were analyzed for valorizing properties and their relationship to lignin structure.

#### Mesoscale Reaction-Diffusion Phenomena Governing Lignin-First Biomass Fractionation.

**Nicholas E. Thornburg**<sup>1</sup>, M. Brennan Pecha<sup>1</sup>, David G. Brandner<sup>2</sup>, Michelle L. Reed<sup>1</sup>, Josh V. Vermaas<sup>1</sup>, William E. Michener<sup>1</sup>, Rui Katahira<sup>1</sup>, Todd B. Vinzant<sup>1</sup>, Thomas D. Foust<sup>1</sup>, Bryon S. Donohoe<sup>1</sup>, Xiaowen Chen<sup>1</sup>, David A. Sievers<sup>1</sup>, Edward J. Wolfrum<sup>1</sup>, Yuriy Román-Leshkov<sup>3</sup>, Peter N. Ciesielski<sup>1</sup>, and Gregg T. Beckham<sup>2</sup>

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Lignin solvolysis from the plant cell wall is the critical first step in lignin depolymerization processes involving whole biomass feedstocks. However, little is known about the coupled reaction kinetics and transport phenomena that govern effective rates of lignin extraction. We will present an experimentally validated simulation framework that determines intrinsic, transport-independent kinetic parameters for the solvolysis of lignin, hemicellulose, and cellulose upon incorporating feedstock characteristics for methanol-based extraction of poplar as an example fractionation process. Lignin fragment diffusion is predicted to compete on the same time and length scales as reactions of lignin within cell walls and longitudinal pores of typical milled particle sizes, with mass transfer resistances predicted to dominate solvolysis of poplar particles exceeding as little as ~2 mm in length. Beyond the ~2 mm threshold, effectiveness factors are predicted below 0.25, implying that pore diffusion resistances may attenuate observable kinetic rate measurements by at least 75% in such cases. Thus, researchers are recommended to conduct kinetic evaluations of lignin-first catalysts using biomass particles smaller than ~0.2 mm in length to avoid feedstock-specific mass transfer limitations in lignin conversion studies. Lastly, this simulation framework will be extended to model the alkaline deacetylation of corn stover, an unrelated pretreatment system which exhibits unique mesoscale diffusion limitations. Overall, this presentation highlights opportunities to improve biomass fractionation and conversion via reaction engineering and provides actionable kinetic information to guide the design and scale-up of emerging biorefinery strategies.

### IMPLICATIONS OF NANOMATERIAL WATER STABILITY FOR DEVELOPING BIOMASS CONVERSION PATHWAYS: THE CASE OF MGO(111) NANOPARTICLES.

**Xiangchen Huo**<sup>1</sup>, Davis Conklin<sup>1</sup>, Mingxia Zhou<sup>2</sup>, Rajeev Assary<sup>2</sup>, Stephen Purdy<sup>3</sup>, Katharine L. Page<sup>3</sup>, Zhenglong Li<sup>3</sup>, Kinga A. Unocic<sup>3</sup>, Raiven Balderas<sup>4</sup>, Ryan M Richards<sup>4</sup>, and Derek Vardon<sup>1</sup> (1)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO, (2)Materials Science Division, Argonne National Laboratory, Lemont, IL, (3)Oak Ridge National Laboratory, Oak Ridge, TN, (4)Colorado School of Mines, Golden, CO

Novel material structures imparting highly active surface sites have gained tremendous research interest due to their potential to enable efficient biomass conversion technologies. However, the high oxygen content of biomass and biointermediates poses unique challenges to catalyst materials. Particularly, oxygen in the form of water is ubiquitous in biomass conversion processes as a feedstock component or a product from oxygen removal chemistries to produce renewable fuels and chemicals. Understanding the impact of water on the stability of material structure and catalytic properties is necessary to inform catalyst development and optimization iterations. This study illustrates the implications of nanomaterial water stability for developing water-forming biomass conversion pathways by methodically examining the evolution of morphological, textural, structural, and surface properties during vapor-phase hydration of MgO(111) nanoparticles under well-controlled conditions in a practical catalytic flow reactor system. MgO(111) nanoparticles possess high surface area and surfaces uniquely terminated by (111) facets, which are characteristic of the advantageous nanomaterials targeted by shape/size controlled synthesis. High activity of fresh MgO(111) nanoparticles was observed for 2-pentanone condensation, an important chemistry to increase boiling point while reducing oxygen content for upgrading biointermediates to heavy-duty and aviation fuels. Computational modeling of the (111) surface reveals the ability of surface hydroxyls to stabilize the low-coordinated surface structure. More importantly, these hydroxyls were shown to mediate proton-transfer elementary steps, hence reducing the thermodynamic barrier for 2-pentanone condensation. While transient water exposure did not significantly affect textural and structural properties, prolonged hydration led to increasing loss of surface area and pore volume coinciding with the appearance of crystalline magnesium hydroxide. Activity for 2pentanone condensation decreased for hydrated MgO(111), which is largely correlated with reduced surface area. Given the observed sensitivity of MgO(111) nanoparticles to water exposure, thermal regeneration was applied and found effective at recovering the material properties and catalytic activity. Overall, our approach of isolating and controlling the factor of interest (e.g., hydration) allows for systematic evaluation of the water stability of nanomaterials and its impact on catalytic performance. This approach can be extended to a wide range of materials to inform catalyst selection and set further optimization targets.

### CATALYTIC FAST PYROLYSIS FOR SUSTAINABLE FUELS AND PRODUCTS.

*Mark R. Nimlos,* Nolan Wilson, and Megan Girdwood Renewable Resources and Enabling Sciences Center, National Renewable Energy Laboratory, Golden, CO

Catalytic fast pyrolysis (CFP) is a versatile conversion technology that can be used to produce liquid transportation fuels, chemicals and materials that have a reduced environmental impact from conventional, fossil-based products. Recent improvements in catalyst formulation and process operation have resulted in higher yield and improved properties of the biocrude from the CFP process. Subsequent separation of the biocrude into liquid fractions allows further processing to form fuels, chemicals, polymers and other carbonaceous materials. Drop-in hydrocarbon fuels are produced by hydrotreating a majority of the biocrude and can help reduce the impact of transportation on climate change by increasing carbon circularity. Other cuts can be separated and used as replacements for existing materials or for novel applications. Oxygenated compounds such as phenol and cresols have been separated from the biocrude and used to synthesize polymer and resins, while others such as 2-cyclopenten-1-one have been isolated and used to prepare novel polymers. Using the existing oxygen functionality found in CFP product molecules reduces the energy demand and greenhouse gas emissions that result from synthesizing these monomers from oxygen-free fossil sources. In some cases, mixtures of phenolic compounds have been isolated from CFP biocrude to prepare biomass-sourced alternatives to conventional insecticides. The phenolics are products of natural decomposition of lignin in the environment and are degraded by existing soil microorganisms unlike many synthesized insecticides, which have problems with environment persistence. Finally, graphite and hard carbon can be prepared from the heavy residues from CFP and can be used as anode material in lithium and sodium ion batteries. Most graphite used for lithium ion batteries is mined and processed using very processes that are very harmful to the environment. As will be discussed in this presentation, the production of fuel and a range of byproducts enables robust biorefinery that not only provides financial resilience, but also reducing the impact of existing petroleum-based fuels and products.

### MODELING AND SIMULATION

### CURRENT PROGRESS AND OPPORTUNITIES ON PROCESS SIMULATION AND CONTROL FOR SUSTAINABILITY USING GREENSCOPE.

### Fernando V. Lima

Department of Chemical and Biomedical Engineering, West Virginia University, Morgantown, WV

Sustainability assessment has become a critical area of research in Process Systems Engineering (PSE) due its paramount importance in various aspects related to achieving economics, energy, and environmental goals. This presentation addresses simulation and control developments in WVU-EPA collaborations associated with sustainability assessment of chemical and energy systems. Such developments involve improvements and applications of the GREENSCOPE (Gauging Reaction Effectiveness for the ENvironmental Sustainability of Chemistries with a multi-Objective Process Evaluator) tool to process systems studies.

A new GREENSCOPE version that is under development at WVU will be presented. This version provides an interface to integrate GREENSCOPE with commercial process simulators (e.g., CHEMCAD), pollution control units (PCUs) for mitigation of air, liquid, and solid releases, as well as life cycle assessment tools. Also, a new visualization tool for 3-D radar plots will be discussed for dynamic sustainability evaluation. These plots are employed for dynamic monitoring and advanced control towards sustainable process operations.

The developed tools will be demonstrated using different applications of chemical and energy systems such as: (i) a fermentation process for bioethanol production; (ii) a biomass/coal-based process for acetic acid manufacturing; and (iii) a biorefinery system using the novel *Opuntia* spp. feedstock. Also, perspectives on future developments will be given to facilitate PSE implementation and improve design, simulation, and control studies for sustainability.

### AN ANALYSIS OF THE RETROFITTING POTENTIAL OF COMMERCIAL AND RESIDENTIAL BUILDINGS IN COLORADO IN ORDER TO REACH EMISSIONS REDUCTION GOALS THROUGH COST-EFFECTIVE MEASURES.

#### Noah Sandoval

*Civil and Environmental Engineering, Colorado School of Mines, National Renewable Energy Laboratory, Golden, CO* 

In 2019, the Colorado Legislature passed House Bill 19-1261 which called for a 90% reduction in greenhouse gas emissions by 2050. In 2017, commercial and residential buildings in Colorado consumed ~40% of all primary energy while producing 40 - 50% of all greenhouse gas emissions. Therefore, it is critical that these building sectors modify emissions to reach this reduction goal. Most commercial and residential buildings have an average lifetime between 50 - 100 years, so the majority of present-day buildings will still be standing in 2050. Thus, the emissions which are attributed to these buildings, which include electrical energy generation and on-site consumption of fossil fuels (e.g. natural gas water heaters and furnaces), will only change with regional energy profiles. One strategy to reduce the emissions of these buildings would be through widespread energy efficiency retrofitting.

The retrofitting of existing buildings to increase their energy efficiency involves two major steps, the assessment of the current condition of a building and future upgrade strategies. This presentation focuses on the first step, attempting to determine the areas of greatest potential for improvement. Colorado has four major climate zones, therefore buildings with similar physical characteristics could have significant differences in their energy loads and end-use profiles. This research will use results from ResStock™ and ComStock™, physics-based, bottom-up models developed by the National Renewable Energy Laboratory to understand the make-up of the commercial and residential building stock in Colorado. From these results, we will compare segments of the building stock with similar characteristics from across the state. From this point, energy retrofitting measures will be simulated to identify what regions in the state have the greatest energy efficiency improvement potential. This analysis can be taken one step further by calculating the most cost-effective energy efficiency solutions by comparing installation costs with lifetime energy savings We will provide localized recommendations for state and local governments on developing a building-sector greenhouse gas emissions reduction strategy for their respective area and comment on the unique challenges and opportunities facing Colorado in mitigating emissions from buildings.

### SYSTEMATIC DESIGN OF SOLVENT RECOVERY PATHWAYS: INTEGRATING ECONOMICS AND ENVIRONMENTAL METRICS.

### **Emmanuel A. Aboagye**, John D. Chea, Austin L. Lehr, Jake P. Stengel, Mariano J. Savelski, Stewart C. Slater, and Kirti M. Yenkie

Chemical Engineering, Rowan University, Glassboro, NJ

Most industrial processes use solvents. Used Solvents end-up in industrial waste streams. Improper disposal of waste streams can have significant environmental impacts<sup>1,2</sup>. Life cycle analysis (LCA) is one of the ways to estimate the environmental impact of a process. LCA quantifies the emissions associated with a product over its entire supply chain, from raw material processing to end-of-use of the product<sup>3</sup>. Another alternative for quantifying the sustainability of a process is the Sustainable Process Index (SPI) methodology<sup>4</sup>. The SPI methodology is an ecological footprint that computes the arable area needed to provide goods and services. SPI is made up of seven footprints, quantified as area. These footprints are area needed for renewable raw material, area needed for non-renewable raw material, area needed to install equipment and infrastructure, area needed for fossil carbon usage, area needed to embed water emissions, soil emissions, and air emissions after the process<sup>4,5</sup>.

Many studies have specifically targeted the economic evaluation of optimal recovery pathways through process selection with the aim of cost minimization. However, there is a need to ensure that these recovery pathways do not pose an additional environmental burden. Thus, sustainability evaluations are needed to make a holistic process selection decision. Multi-objective optimization approaches, which implement several objective functions, are one of the ways to quantify the economics and sustainability of a recovery process simultaneously<sup>6</sup>. Chea et al (2020)<sup>7</sup> have previously worked on the economic feasibility of the solvent recovery process. This work presents an extension of this previous work done by Chea et al. (2020) by incorporating sustainability matrices into the solvent recovery process. Thus, we integrated mathematical models that quantified the SPI of each recovery technology besides economics. We formulated a multi-objective optimization problem for minimizing the costs as well as the ecological footprint. Additionally, we estimated the greenhouse gas (GHG) emissions associated with each recovery pathway.

### **DEM MODELING APPLICATION TO BIOMASS - OVERCOMING HANDLING PROBLEMS.**

### **Carrie Hartford**

Engineering, Jenike & Johanson, Inc., San Luis Obispo, CA

While the science of biogas conversion and bio-refining is developing at a rapid pace, pilot and commercial plants struggle with reliably feeding a range of biomass materials to the plant. Biomass does not flow like a liquid or dry sand and needs to have handling equipment design according to the flowability of the feedstock taking into consideration all material properties such as friction, bridging tendencies, bulk density, particle size distribution, aspect ratio, moisture content, edge cuts, impurities, etc. This talk will discuss the key technical and economic challenges related to scale-up and biomass material handling and the steps required to overcome those challenges. Discrete Element Method (DEM) modeling and its application to biomass will be discussed. Various examples, pictures and case studies will be discussed throughout the presentation.

### CIRCULAR ECONOMY LIFECYCLE ASSESSMENT AND VISUALIZATION (CELAVI): A New Hybrid Multi-Scale Dynamic Model for Assessing Circularity Transitions.

**Rebecca Hanes**<sup>1</sup>, Tapajyoti Ghosh<sup>1</sup>, Alicia Key<sup>2</sup>, and Annika Eberle<sup>1</sup> (1)Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO, (2)National Wind Technology Center, National Renewable Energy Laboratory, Golden, CO

Developing a circular economy is widely anticipated to produce societal, environmental, and economic benefits, but it is unlikely that these benefits will be distributed equally across industrial sectors and across regions. Furthermore, some negative externalities could result from a circular transition. Methods such as life cycle assessment and partial or general equilibrium models have been widely used to assess the impacts of linear systems; to a lesser extent, these methods have been applied to assess circular systems. We argue that modeling circular systems requires capabilities beyond what any single previously developed method offers and present our hybridized modeling framework, which is being developed to assess how impacts vary as system circularity increases.

Our Circular Economy Lifecycle Assessment and Visualization (CELAVI) framework is multi-scale, regionalized, and dynamic and is being developed with a primary focus on energy materials and technologies. The CELAVI framework represents the economic and technological changes involved in a linear-to-circular transition along with the associated societal and environmental externalities. It captures selected energy technology supply chains using detailed, dynamic models of production, use, and circular pathways. These supply chain models are linked to background life cycle processes which may be dynamic or static, and which can be represented at several levels of aggregation, depending on how impactful each background process is relative to the overall system. We intend the framework for use in decision support by governing bodies, corporations and non-government organizations who are working towards a circular economy at local, regional, and national levels.

In this presentation we describe the strengths and weaknesses of previous circular economy modeling efforts and review the capabilities of the CELAVI framework. We also discuss a use case in which wind turbine circularity is modeled over time. We focus on turbine blades, for which recycling and other circular pathways are still under development. We examine how the circularity of turbine components might change over time as technology costs evolve through learning-by-doing and applied research, and show how spatial considerations such as the locations of wind farms and landfills can influence wind turbine supply chain externalities and thereby inform circular decision-making.

### Tuesday, August 4th, 2020

### **KEYNOTE**

### A BIG PICTURE TREATISE TO SUSTAINABLE DEVELOPMENT AND INNOVATION.

### Minal Mistry

Materials Management, Oregon DEQ, Portland, OR

A big picture treatise to sustainable development and innovation. This will take shape by highlighting prevailing systems level myths and connecting them to planetary boundaries and material consumption realities. We will draw upon the state's detailed GHG inventories over the past 20 years to illustrate the message. The second part of the presentation will ask what might innovation look like if we change the approach from growth expansion to well-being expansion.

Leveraging Sustainability Regarding Plastic: Law and Policy Landscape.

### **DESIGN FOR CIRCULARITY**

### **DESIGN FOR CIRCULAR ECONOMY AND CONVERGENCE RESEARCH.**

#### Melissa M. Bilec

University of Pittsburgh, Pittsburgh, PA

The current consumption model is linear: (1) acquire raw materials, (2) produce and use goods, and then (3) dispose of them. This 'take, make, waste' model has dominated the global economy for hundreds of years. Today, however, coupling this linear model with growing population and affluence around the world has led to serious unintended global consequences. Cumulatively, global extraction of construction minerals exceeds 10 billion metric tons each year, representing the fastest growth rate in any sector over the past century. In contrast to the linear model, a circular economy (CE) aims to decouple economic growth from resource consumption by cycling products and materials back into production, either by returning materials to generate new products, or by releasing benign substances to the environment through degradation.

Since the built environment sector is responsible for a major share of carbon emissions, resource use, and waste streams across the globe, CE can offer strategies to mitigate the impacts. Despite the urgency of the matter, the building sector is falling behind on circular economy research and development. This talk discusses the latest efforts and the knowledge gaps about the circular economy in the built environment. The authors performed a bibliometric analysis on 2,000 recent publications on circular economy to answer questions like "what disciplines are involved in the current discussion on CE and the built environment?", "what countries and institutions are leading research in circular building design?", and "what are the recurrent themes in the literature and what remains unexplored?". The results from the analysis are vital to 1) identifying potential collaboration among CE stakeholders; 2) discussing the contextual differences between the countries involved in CE research for the built environment, and 3) highlighting the main opportunities for future research on the CE and the built environment.

### SYNTHESIS AND CHARACTERIZATION OF LIGNIN-GRAFTED-POLY(E-CAPROLACTONE) FROM DIFFERENT

### **BIOMASS SOURCES.**

### *Mi Li*<sup>1</sup> and Arthur J. Ragauskas<sup>2</sup>

### (1)Forestry, Wildlife and Fisheries, University of Tennessee, Knowxville, TN, (2)Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN

Modification of lignin with poly(*e*-caprolactone) is a promising approach to valorize industrial low-value lignins and to advance the bioeconomy. We have synthesized lignin grafted poly(*e*-caprolactone) (lignin-*g*-PCL) copolymers *via* ring-opening polymerization of *e*-caprolactone with different types of lignins varying on botanical sources (i.e., G-type pine lignin, S/G-type poplar lignin, and C-type *Vanilla* seeds lignin) and lignin extraction methods (Kraft and ethanol organosolv pulping). The lignin-*g*-PCL showed remarkably improved compatibility and dispersion in acetone, chloroform, and toluene in comparison to non-modified lignins. The structure and thermal properties of the lignin-*g*-PCL were investigated using FTIR, <sup>31</sup>P NMR, 2D HSQC NMR, GPC, and DSC. We have found that all the technical lignins are reactive to the copolymerization reaction regardless of their plant source and isolation methods. The molecular weights of the synthesized lignin-*g*-PCL copolymers are positively correlated with the content of aliphatic lignin hydroxyls as the copolymerization reaction tends to occur preferentially at the aliphatic hydroxyls than the phenolic hydroxyls of lignin. Thermal analyses of the lignin-*g*-PCL copolymers were studied, and in general, a reduction of melting temperature and crystallinity percentage in comparison to the neat PCL was observed. However, the thermal behavior of lignin-*g*-PCL copolymers varies depending on the lignin feedstocks employed in the copolymerization reaction. In addition, we have found that the lignin-*g*-PCL can be chemically recycled to the original *e*-caprolactone that can be used infinitely.

### **DESIGN AND PROCUREMENT CONSIDERATION FOR EOL ASPIRATIONS.**

#### Peter Canepa

Materials Management, Oregon DEQ, Portland, OR

Design for sustainability is commonly realized in simplified material attributes such as using recycled or bio-based materials, or designing for end of use treatment preference such as recyclability or compostability. This presentation will speak to prevailing discourse about single-use packaging sustainability. It will highlight our recently published research that drew up nearly two decades of LCA data to establish the efficacy of simplified attributes' ability to predict lower environmental impact materials. The significance of this research affects how materials are developed, how perceived material criteria are used in design and purchasing decision to lower actual environmental impacts.

**GLOBAL PLASTIC TRADE: IMPLICATIONS FOR ENVIRONMENTAL SUSTAINABILITY AND CIRCULARITY.** 

#### Vikas Khanna

### Civil and Environmental Engineering, University of Pittsburgh, Pittsburgh, PA

Plastics have exponentially increased in popularity from their commercialization in the 1950s. 2 million metric tons of plastic were produced globally in 1950, compared to around 350 million metric tons in 2018 (Geyer 2017, Plastics Europe 2019). Plastics are ubiquitous and used in a variety of consumer and industrial products. Simultaneously, the quantity of plastic waste generated globally has increased significantly over the past few decades, with sustainable end-of-life management remaining prohibitively expensive or unavailable in many regions. Tracing the global flows of plastic products using systems-based analysis is a key step towards enabling circular economy of plastics. This talk will describe our efforts on developing a network model of global plastic trade with a focus on thermoplastics. The model could serve as a starting point for implementing circular economy by identifying opportunities to improve circularity in the plastic economy for different parts of the world through detailed understanding of their plastic production and consumption patterns. Several network analysis based measures are used to identify the critical nodes and understand pattern of interconnections and dependencies within the network. Additionally, the model is utilized to quantify the energy and greenhouse gas emissions embodied in global plastic trade. The evolution of the plastics trade network and its implications for managing end-of-life plastic waste and developing circular economy of plastics will be described.

### SOCIO-TECHNICAL ANALYSIS OF PHOTOVOLTAICS END OF LIFE MANAGEMENT: AN AGENT-BASED MODELING APPROACH.

Julien Walzberg<sup>1</sup>, Alberta Carpenter<sup>2</sup>, and Garvin Heath<sup>3</sup>

(1)National Renewable Energy Laboratory, -1, CO, (2)Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO, (3)Strategic Energy Analysis Center, National Renewable Energy Laboratory (NREL), Golden, CO

The circular economy (CE) is an umbrella concept proposing to tackle environmental and resource scarcity issues by maximizing value retention in the economy. The concept implies to reduce the use of materials, reuse products and their components and recycling. A growing demand for renewables and energy storage technologies is raising concerns over the availability of scarce materials such as silver, lithium and neodymium. For instance, demand for photovoltaics (PV) materials could increase by 3000% between 2015 and 2060. Applying CE concept to renewables such as PV could therefore alleviate the issue of resource scarcity while providing economic benefits.

Transitioning to a CE implies changes in complex global supply chains. Businesses and consumers are expected to take part in new business models such as the sharing economy. In this context, quantitative sustainability assessment of circular economy strategies may require accounting for behavior change, a requirement that methods from complex system science such as agent-based modeling meet. Thus, we proposed an agent-based modeling approach to assess CE strategies and apply it to study circularity in the PV supply chain. Four different types of agents are represented (PV owners, installers, recyclers, and manufacturers) and five possible end-of life pathways – including three CE strategies – are modeled. Drawing from the literature, agents' behavior rules include the generation of waste, PV purchase and end-of-life management decisions and are based on techno-economic factors as well as social factors.

Results show that techno-economic and market levers may be used to spur circularity of the PV supply (e.g., improved recycling processes or warranties for used modules). Lower recycling fees born by PV owners and installers improves recycling rate by roughly 1.1% for each dollar decrease of the recycling fees. Moreover, a scenario with improved warranties for used PV modules improves the reuse rate by more than three times reaching 6.5%. However, the recycling rate is halved in that scenario because the reuse and recycling pathways competes in agent's decisions. Finally, combining different levers (e.g., lower recycling fees with higher landfill fees) may prove the most efficient strategy to maximize the circularity of the PV supply chain.

### END-OF-USE (LIFE) OF GOODS (PRODUCTS

### DATA-DRIVEN FRAMEWORK FOR TRACKING CHEMICAL FLOWS AT END-OF-LIFE STAGE.

Jose D. Hernandez-Betancur<sup>1,2</sup>, Mariano Martín<sup>1</sup>, and Gerardo J. Ruiz-Mercado<sup>3</sup> (1)Department of Chemical Engineering, University of Salamanca, Salamanca, Spain, (2)ORISE Postmaster, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH, (3)Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH

Determining whether a chemical may represent an unreasonable risk to the health of a human being and the environment is an important criterion for an adequate choice of materials for use, consumption, and regulatory decision-making. For example, the U.S. Environmental Protection Agency (USEPA) needs to assess the risk of chemicals under the Toxic Substances Control Act (TSCA), like those implemented by the European Chemicals Agency (ECHA) under the Registration, Evaluation, Authorization, and Restriction of Chemicals (REACH). However, assessing risk at end-of-life (EoL) stage is a time-consuming and challenging task due to data collection, manipulation, availability, uncertainty, and traceability. Therefore, this work aids by supplying a big data engineering framework, based on publicly-available regulatory databases, for tracking a chemical in waste streams generated at a given industrial facility and then transferred to off-site locations for further management, where other releases from pollution abatement technologies may occur. The proposed approach is expected to be useful to streamline chemical risk and exposure assessment at EoL stage, considering statistical techniques, process simulation, and build learning-from-data models to predict releases of existing or new chemicals. In addition, this framework may support life cycle initiatives by supplying inventories of chemical releases from EoL activities and integrating life cycle assessment and risk analysis at EoL scenarios.

Disclaimer: The views expressed in this abstract are those of the authors and do not necessarily represent the views or policies of the USEPA.

### **RECOVERY OF CATHODE MATERIALS FROM SPENT LITHIUM-ION BATTERIES USING MOLTEN SALT SYSTEMS.** *Yi Ji*<sup>1</sup>, *Edwin Kpodzro*<sup>2</sup>, *Chad T. Jafvert*<sup>3</sup>, *and Fu Zhao*<sup>4</sup>

(1)Environmental and Ecological Engineering, Purdue University, West Lafayette, IN, (2)Mechanical Engineering, Purdue University, West Lafayette, IN, (3)Lyles School of Civil Engineering/Environmental and Ecological Engineering, Purdue University, West Lafayette, IN, (4)Mechanical Engineering/Environmental and Ecological Engineering, Purdue University, West Lafayette, IN

Driven by the growth of the electric vehicle market, demand for lithium-ion batteries (LIBs) is expected to increase significantly in the next decade. Meeting this increasing demand requires sufficient supply of some critical materials such as cobalt, nickel, and manganese needed to make cathodes. Recycling of spent LIBs can play an important role in mitigating the supply risk. Traditional hydrometallurgical methods which use acids to leach out metals are not desirable due to cost and environmental concerns. Moreover, additional precipitation and re-synthesis processes are required to make new cathodes. Recently cathode-to-cathode or direct recycling has attracted interest, which aims at recovering materials from used cathodes such that the recovered materials can be used to make new cathodes with minimal treatments. The challenges come from the strong binding force provided by polyvinylidene fluoride (PVDF) binder among the particles of cathode materials and between the cathode layer and the current collector, as well as concerns on the release of fluorine containing compounds. A promising direct recycling approach is to use molten salts to decompose or deactivate PVDF while absorbing fluorine emissions.

In this study, molten salt systems are explored to recover heterogeneous active materials (lithium nickel manganese cobalt oxide and lithium manganese oxide). Different molten salt systems are compared: AlCl<sub>3</sub>-NaCl system, lithium hydroxide-lithium nitrate (LiOH-LiNO<sub>3</sub>) system, and lithium acetate-lithium nitrate (LiOAc-LiNO<sub>3</sub>) system. Scanning electron microscopy (SEM) images show that the surface morphology after lithium salt treatments has minimal changes on crystal structure. The recycled products from the LiOAc-LiNO<sub>3</sub> system have reduced particle size with spherical shapes. The X-ray photoelectron spectrometer (XPS) results indicate the decomposition of PVDF. In contrast, PVDF has a physical change to delaminate cathode materials in LiOH-LiNO<sub>3</sub> system. Large agglomerates are observed via SEM. Effects of temperature, salt-to-cathode electrode mass ratio, and heating time on recovery efficiency are also investigated.

### WASTE TO ENERGY (FUEL OR POWER)

### WET WASTE FOR SUSTAINABLE AVIATION FUEL.

**Derek Vardon**<sup>1</sup>, Nabila Huq<sup>1</sup>, Glenn Hafenstine<sup>1</sup>, Xiangchen Huo<sup>1</sup>, Davis Conklin<sup>1</sup>, Stephen Tifft<sup>1</sup>, Jim Stunkel<sup>1</sup>, Daniela Stück<sup>1</sup>, Hannah Nguyen<sup>1</sup>, Earl Christensen<sup>2</sup>, Gina Fioroni<sup>3</sup>, Matthew Wiatrowski<sup>1</sup>, Yimin Zhang<sup>4</sup>, Ling Tao<sup>1</sup>, and Zia Abdullah<sup>1</sup>

(1)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO, (2)Transportation Technologies, National Renewable Energy Laboratory, Golden, CO, (3)Integrated Mobility Science, National Renewable Energy Laboratory, Golden, CO, (4)Strategic Energy Analysis Center, National Renewable Energy Laboratory (NREL), Golden, CO

With the increasing demand for low-carbon sustainable aviation fuels (SAF), new conversion technologies are needed that can economically expand current U.S. feedstock supplies while meeting carbon intensity reduction targets. Wet waste is one such promising low-cost, widely available feedstock with the energy potential to displace over 20% of U.S. jet fuel consumption; however, the complexity and high moisture of wet waste typically relegates its embedded energy to methane production from anaerobic digestion. To overcome this limitation, this talk will discuss recent efforts at NREL to catalytically upgrade C2-C8 volatile fatty acids (VFAs) derived from arrested anaerobic digestion into SAF that is suitable for blending into conventional aviation fuels. Findings will be presented in regard to: i) challenges and opportunities when using wet-waste derived VFAs for aviation fuel production, ii) catalytic conversion pathway and performance studies when upgrading model and wet waste VFAs, iii) neat and blended VFA-SAF fuel property testing results to meet ASTM jet fuel specifications, and iv) techno-economic and life cycle analysis considerations to guide further process R&D. Overall, this talk will provide a comprehensive look at the potential of wet waste-derived VFA-SAF from a catalytic conversion viability and jet fuel property standpoint.

### SUSTAINABLE ENERGY FROM BIOMASS AND WASTES THE TAYLOR GASIFICATION PROCESS.

#### Mark A. Paisley

Taylor Biomass Energy LLC, Montgomery, NY

The uncertain future for fossil fuels coupled with an increasing desire to provide sustainable, renewable energy supplies has led to renewed interest in a number of alternative fuel sources. Biomass gasification can provide a renewable basis for supplying electric power as well as a broad suite of chemicals such as Fisher-Tropsch liquids or hydrogen from sustainable resources. The Taylor gasification process, being developed by Taylor Biomass Energy is a biomass gasification process that produces a MCV gas. The Taylor gasification process provides improvements over currently available gasification processes by integrating improvements to reduce issues with ash agglomeration and provide in-situ destruction of condensable hydrocarbons (tars), an essential element in gas cleanup. The gas conditional synthesis gas and to adjust the composition of the synthesis gas. Taylor Biomass Energy has integrated this unique gasification process with a well-developed sorting and recycling process that can produce a clean feedstock for energy recovery from abundant, sustainable residue materials such as construction and demolition residuals and MSW. The combination of this sorting and separating process with the Taylor Gasifier provides sustainable energy from materials that would otherwise be discarded.

Construction is underway on an integrated combined cycle power system incorporating the Taylor Gasification Process and utilizing biomass feedstocks recovered from municipal solid wastes (MSW) and construction and demolition wastes C&D). The Taylor Recycling Facility, LLC, located approximately 70 miles northwest of New York City in Montgomery, NY, is a leader in C&D and waste wood recycling. The integrated process will include a full gas turbine based combined cycle system, connection into the New York ISO, and identification of renewable energy credit options. The Taylor Gasification Process, its modular design, and implementation into the commercial IGCC system in Montgomery, NY is discussed.

### CHEMICAL RECYCLING OF WASTE PLASTIC FOR THE PRODUCTION OF USEFUL CHEMICALS.

### Mohammed A Awwad Sr.

chemical engineering, KFUPM, daharan, Saudi Arabia

The extent of plastics use in everyday life is evident by the fact that the annual global plastic production has exceeded 350 million tons. Most of the plastic materials ends up in landfills after their use and approximately 3 % of global plastic production has littered the oceans causing negative impacts on the environment and marine life. The projected continuous increase in the production of plastics due to their versatile applications also represents an economic opportunity by recycling them while addressing the adverse environmental concerns. Currently employed mechanical recycling techniques have limitations because of poorer product quality after each cycle. Hence, chemical recycling of plastic waste has been an active area of research recently.

In this study, the thermochemical plastic recycling processes namely, gasification has been investigated for the production of important feedstock chemicals. This work explored the gasification of various waste plastics for recycling and evaluated them qualitatively and in terms of process efficiency. The results show that among various plastic waste composites, mixture of PE+PET require the least amount of energy for the thermochemical breakdown with high concentration of CO2 in the reactor effluent. On the other hand, the mixture of PE+PS showed reasonable amount of syngas from the gasification process

### ADVANCED RECYCLING TECHNOLOGIES

### ECONOMIC IMPACT OF YIELD AND COMPOSITION VARIATION IN BIOENERGY CROPS: POPULUS TRICHOCARPA.

Renee Happs<sup>1</sup>, Andrew Bartling<sup>1</sup>, Crissa Doeppke<sup>2</sup>, Anne E. Harman-Ware<sup>2</sup>, Robin Clark<sup>3</sup>, Erin Webb<sup>4</sup>, Mary Biddy<sup>1</sup>, Jin-Gui Chen<sup>3</sup>, Wellington Muchero<sup>5</sup>, Gerald A. Tuskan<sup>5</sup>, and **Brian H. Davison**<sup>6</sup> (1)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO, (2)Biosciences Center, National Renewable Energy Laboratory, Golden, CO, (3)Oak Ridge National Laboratory, Oak Ridge, TN, (4)Oak Ridge National Laboratory, (5)Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (6)Biosciences Division, BioEnergy Science Center and Oak Ridge National Laboratory, Oak Ridge, TN

To achieve a bio-based economy, it is necessary to consider variability within a feedstock population. One aspect of this is to consider both feedstock and conversion costs for perennial biofeedstocks. We must understand the range of key phenotypic characteristics when selecting economically advantageous genotypes for domestication in an optimized supply chain. In this analysis, we measured cell wall composition traits in a large natural variant population of *Populus trichocarpa*. The results were combined with agronomic growth data from the matching genotype to conduct various techno-economic analyses, evaluating the impacts of physical and compositional variability and determining the ultimate phenotypic drivers for yield and economic metrics. As a first step, we only considered carbohydrate composition as the primary measure of quality, because of its direct relation to final fuel (i.e., ethanol) yield. We show that while ethanol yield per land area per year and minimum fuel selling price were most strongly impacted by tree size; when considering the largest 25% of trees, size and carbohydrate content were nearly identical influencers on minimal fuel selling price, highlighting the need to focus on both size and carbohydrate content in selecting economically optimal feedstocks.

The development of a sustainable bio-based economy for renewable carbon for fuels, chemicals and materials remains an important research area. This work presents a complete analysis on how to "value" both feedstock yield and feedstock conversion quality. The biorefinery industry frequently has stated that high quality feedstocks are desired but has not been able to put a value to quality compared to the major driver of yield. The significance is that it allows both feedstock and conversion researchers to begin to interact on the quality of the feedstock provided to a biorefinery.

### CHEMICAL UPCYCLING OF POLYETHYLENE WASTE INTO NEW POLYMERS.

*Jennifer Le Roy BioCellection, Menlo Park, CA* 

Over 90% of plastic waste ends up in a landfill, incinerators, or oceans. Mechanical recycling technologies are one possible solution to managing plastic waste, yet polyethylene film remains a major recycling challenge. Most chemical recycling technologies focus on depolymerizing commodity plastics back into their original monomers. However, what if the carbon rich backbone of polyethylene can be broken down to make more valuable and versatile monomers than ethylene. This is our vision at BioCellection Inc. We have developed an Accelerated Thermal Oxidative Decomposition (ATOD<sup>™</sup>) process where polyethylene is rapidly oxidized into lower molecular weight species. These valuable organic compounds are harvested, purified, and used to make new polymer products. This talk will cover how we are using chemical building blocks from decomposed polyethylene to create new, high-performing polymers.

### THE REALITIES OF RECYCLING PACKAGING FOAM.

#### Darren Post

Expandable Styrenics, NOVA Chemicals, Monaca, PA

There are many misconceptions about the recyclability of foam packaging cushions. In reality, foam parts are being recycled every day. There are many solutions for thermoplastic foams. Foam packaging cushions are reground and molded back into foam cushions and they are extruded into various solid products. The two financial challenges for consumers is wanting to recycle foam is the logistics of getting light weight foam cushions to a location where they can be used, or the cost of sorting mixed stream recycling at a recycling facility. This presentation will include cost effective options and examples of successful recycle solutions. It will also provide an update on the industries activities to reduce ocean plastic waste.

### THINKING OUTSIDE THE CIRCLE: CREATING NOVEL MATERIALS AND BIGGER MARKETS FOR POST-USE PLASTICS THROUGH ADVANCED RECYCLING.

### Ben Scott

GreenMantra Technologies, Brantford, ON, Canada

A single-use plastic (SUP) bag has an estimated lifespan of 12 minutes. A plastic straw is typically used for less than 20 minutes. A full circle can be created by reusing that discarded plastic bag or straw to make a new SUP item... and by doing so, another 12 or 20 minutes of usefulness can be derived from the resource. This SUP-to-SUP circle achieved by traditional mechanical recycling can typically be completed only a limited number of times before plastic quality is diminished and insufficient for further processing.

What if we could expand the useful lifespan of plastic from these discarded plastic items to 20 years instead of 20 minutes? The novel chemical recycling technology designed by GreenMantra does exactly that. This technology takes advantage of the integrity of the plastic molecule to create new high-value materials that are used as performance additives in various industrial applications. Some of the largest use cases are in construction infrastructure applications that have useful lifespans of 20-50 years.

GreenMantra's business model is not seeking to create a perfect circle. Instead, it bridges new circles together to expand the lifespan and applicable end markets for discarded plastics. By "thinking outside the circle", GreenMantra has successfully scaled chemical recycling businesses and are diverting tens of thousands of pounds of plastic from our environment into new applications each year. This presentation will give an overview of GreenMantra's technology and the business model that has allowed the company to become one of the first companies to fully scale an advanced recycling business.

### WASTE VALORIZATION (PLASTICS AND MORE)

### QUALITY IMPROVEMENT OF POST CONSUMER RECYCLED MATERIALS.

### **Craig Gorin** Dow, Midland, MI

Post-consumer recycled materials remain underutilized industrially due to issues of "poor quality". Key challenges include the need for separation of desired materials from complex formulations or multilayer structures, and the presence of contaminants causing poor organoleptics, aesthetics or mechanical performance. An exploration of potential options to enable quality improvement will be presented, using polyethylene and polyurethane waste as examples.

### TACKLING THE WASTE PLASTICS PROBLEM – PLASTICS SUPPLY-CHAIN MODELING AND CHEMICAL CATALYSIS EFFORTS IN THE BOTTLE CONSORTIUM.

**Lucas D. Ellis**<sup>1</sup>, Scott Nicholson<sup>2</sup>, Nicholas A. Rorrer<sup>1</sup>, Sara Orski<sup>3</sup>, Yuriy Román-Leshkov<sup>4</sup>, Alberta Carpenter<sup>2</sup>, Kathryn L. Beers<sup>5</sup>, and Gregg T. Beckham<sup>1</sup>

(1)Renewable Resources and Enabling Sciences Center, National Renewable Energy Laboratory, Golden, CO, (2)Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO, (3)NIST, Gaithersburg, MD, (4)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, (5)National Institute of Standards and Technology, Gaithersburg, MD

Over eight billion metric tons of plastic have been created between 1950-2015, and this figure is expected to double in the next three decades. Accumulation of plastic in our landfills, waterways, and oceans, whether in the form of plastic bags, micro-plastics, or other waste, is becoming a critical issue. Today's recycling technology is not capable of solving this problem. New technologies, developed through fundamental research, are thus required to develop robust and cost-competitive recycling strategies, or upcycling, to further the circular economy. A newly developed consortium has formed to deliver on this ambition with a goal of developing selective and scalable technologies that enable cost-effective recycling, upcycling, and increased energy efficiency. Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment (BOTTLE<sup>™</sup>, www.bottle.org) is a research consortium, supported by the U.S. Department of Energy's Bioenergy Technologies Office and the Advanced Manufacturing Office. In this talk, I will introduce the BOTTLE consortium, outlining our vision, mission, and goals, and present a deep dive into two projects within this research umbrella.

First, I will outline our efforts to estimate the supply chain energy requirements and greenhouse gas emissions associated with industrial consumption of synthetic plastics in the U.S. Overall, this work establishes a baseline for comparison of tomorrow's disruptive chemical recycling technologies and bio-based plastics relative to today's incumbent petroleum-derived polymers.

Secondly, I will describe our work to improve on a recently developed dual catalytic system for low temperature depolymerization of polyethylene (PE) to liquid alkanes at temperature below 200°C, without the need for reactive gases like hydrogen. Previous work has demonstrated this technology with homogeneous catalysts, such as iridium pincers. In this work, we sought to develop and explore a variety of robust heterogeneous dehydrogenation and olefin cross metathesis catalytic systems to maximize reactivity in the depolymerization of PE. Our best catalytic system is capable of >70% conversion of 1 g of n-eicosane in 15 hr at 200°C, resulting in a distribution of alkane products ( $C_6$ ,  $C_7$ ,  $C_8$ , etc.). We applied these systems to PE substrates resulting in a >75% reduction in molecular weight of the original polymer.

### A WEDGE-BASED APPROACH TO MODELING POTENTIAL CIRCULAR ECONOMY SOLUTIONS FOR PLASTIC WASTE STREAMS.

#### **Scott Nicholson**, Arpit Bhatt, Colin McMillan, and Alberta Carpenter Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO

Of the 35 million tons of plastic waste present in US municipal solid waste streams in 2017, an estimated 74% was sent to landfill, with the balance being either combusted for energy recovery (16%) or recycled (8%) <sup>[1]</sup>. In this work, we employ a wedge-based analysis framework to understand the potential for a range of technologies to handle the growing landfilled plastic waste stream by estimating material, energy, and greenhouse gas impacts from several separation/recycling/upcycling technologies, including triboelectrostatic separation <sup>[2]</sup>, polyvinyl chloride (PVC) solvent extraction <sup>[3]</sup>, polyethylene terephthalate (PET) upcycling to composites [4], and others. The wedge analysis approach was established in the seminal 2004 paper by Pacala and Socolow <sup>[5]</sup>, which focused originally on climate stabilization via greenhouse gas (GHG) emission reductions. Here, the wedge framework is generalized to account for 1) metrics beyond GHG emissions, including material diversion from landfill and energy requirements, and 2) non-linear technology adoption trajectories unique to each of the referenced technologies <sup>[6]</sup>. Preliminary results will be presented as a case study within an ongoing "circular economy" study being conducted by the Strategic Analysis group of the US Dept. of Energy Advanced Manufacturing Office.

### Wednesday, August 5<sup>th</sup>, 2020

### SUSTAINABLE PROCESS DESIGN

SUSTAINABILITY IN THE CHEMICAL PROCESS INDUSTRIES THROUGH PROCESS INTENSIFICATION AND MODULAR MANUFACTURING.

**Paul Yelvington<sup>1</sup>** and Ignasi Palou-Rivera<sup>2</sup> (1)AIChE, New York, NY, (2)RAPID, New York, NY

The manufacturing sector accounts for a quarter of the total U.S. energy use, and the process industries (chemicals, petroleum refining, pulp and paper, iron and steel) are the largest energy consumers in the sector. Likewise, these industries significantly impact other dimensions of sustainability including water use, climate change, clean energy, waste management, and human health. Process intensification (PI) is an often radical rethinking of chemical processes to remove bottlenecks, improving productivity and safety while reducing waste, energy consumption, production cost, and carbon footprint. PI is often a shift from the conventional "unit operations" paradigm in chemical processing to a more integrative paradigm. Modular manufacturing, a complementary concept, is an approach to building chemical plants that favors assembly of pre-fabricated, standardized modules rather than conventional "stick-built" construction. Modular manufacturing also provides opportunities for distributed chemical manufacturing that utilizes stranded resources such as waste biomass feedstocks or renewable wind and solar power. Modular manufacturing also enables a shift from the bigger-is-better paradigm in chemical production to a small, modular paradigm where economies of scale are replaced with economies of mass production. Both PI and modular manufacturing are tools that can be used to improve the sustainability of the chemical process industries, which are under pressure to change given recent shifts in supply and demand, the rise of inexpensive renewable power, and an increased need to reduce operational footprints. Our work uses research and education to promote better process technologies and to define appropriate metrics to capture the impact of these technologies on productivity and sustainability.

### SUSTAINABLE SOCIAL-ECOLOGICAL SYSTEMS

### WHAT WOULD IT TAKE FOR A UNIVERSITY CAMPUS TO BE FULLY ELECTRIFIED AND CARBON NEUTRAL? A TECHNO-ECONOMIC ANALYSIS FOR THE UNIVERSITY OF DAYTON CAMPUS.

Ryan P. Shea<sup>1</sup>, Matthew O. Worsham<sup>2</sup>, Andrew D. Chiasson<sup>3</sup>, Kelly Kissock<sup>3</sup>, and **Benjamin J. McCall**<sup>4,5</sup> (1)Rocky Mountain Institute, Boulder, CO, (2)Facilities Management, University of Dayton, Dayton, OH, (3)Department of Mechanical and Aerospace Engineering, University of Dayton, Dayton, OH, (4)Hanley Sustainability Institute, University of Dayton, Dayton, OH, (5)Departments of Physics and Chemistry, University of Dayton, Dayton, OH

This presentation analyzes the cost-effectiveness of converting the University of Dayton (UD) to a fully-electrified, renewably powered, carbon-neutral campus by 2025. The greenhouse gas (GHG) impact and 30-year lifecycle costs (LCC) of a scenario including four primary strategies for transitioning to carbon-neutrality were analyzed; scaling building energy efficiency was determined to reduce GHG emissions by 12% with \$10 million LCC savings from business as usual, switching the campus fleet to electric vehicles would reduce GHG emissions by 0.4% with \$2 million LCC savings, switching from on-site natural gas combustion to geothermal heat pumps would reduce GHG emissions by 15% with a \$15.5 million LCC premium, and procuring renewable electricity through a power purchase agreement with a new-build renewable generator would eliminate the remaining 73% of GHG emissions with a \$1.7 million LCC premium. In total, achieving a carbon-neutral campus would increase the 30-year LCC of UD's energy systems by 2.4%, from \$211.8 million to \$216.9 million. This is likely a reasonable investment to consider, given the uncertainties in future commodity pricing, the potential of future regulatory mechanisms like carbon pricing that would internalize the social cost of carbon, and the urgent need to reduce global GHG emissions.

### SUSTAINABILITY: A GOAL OR A SYSTEM'S STATE?

### Michael Ben-Eli

The Sustainability Laboratory, New York City, NY

A systems perspective will be used to discuss the concept of sustainability. From this perspective, sustainability can be regarded as a particular system's state that is driven by specific, underlying structures. This view is fundamentally different than one regarding sustainability merely as a normative goal, as it is presently regarded by most.

Insight into the kinds of structures that mediate a system's state open the door to proactive design and novel rewiring of new structures and mechanisms—social, economic, technology-related, and others—that are necessary for yielding effective change. In this case, promoting the sustainability agenda and establishing the concept of sustainability as the organizing principle on the planet.

The kind of change required to transform the prevailing trajectory of human affairs is presented as a second-order change: a change that calls for a major shift and a complete transformation of the system itself, not merely in a few aspects of its behavior.

In this context, a new definition of sustainability is offered, from which five core sustainability principles are derived, along with their respective policy and operational implications. Together, these principles prescribe the conditions that must be met to attain sustainability as an enduring state.

### INNOVATION FOR SUSTAINABLE BUSINESSES AND INDUSTRIES

#### **INNOVATIONS AND REGULATIONS FOR BIOBASED AND SUSTAINABLE LUBRICANTS.**

#### Mark Miller

Biosynthetic Technologies, Indianapolis, IN; Business, Ramapo College of New Jersey, Ramapo, NJ

Green initiatives are everywhere. Bio-fuels, wind energy, renewable fibers are just a few of the environmental initiatives that have recently made headlines. Meanwhile some of the greatest innovations have been in the development and utilization of high performance, environmentally acceptable lubricants (EALs). This paper/presentation focuses on the innovations, features, benefits, strengths and limitation of the different types of EALs. It explores classification of base fluids and additives as well as the requirements of finished lubricants. It compares the performance of conventional petroleum products and biolubricants. The different definitions of environmental acceptability why that is important will be explored. The regulatory driving forces will be identified as well as the requirements for each. The considerations for choosing the type of EAL that is most applicable to specific applications will be studied. Finally, the best maintenance practices to ensure long fluid and equipment life will be discussed.

DECARBONIZATION

#### **ORGANIC WASTE FROM LIABILITY TO A CARBON NEGATIVE RENEWABLE FUEL.**

#### Alexandros N. Karaiskakis

Science, Technology and Business Innovation, Bioenergy Devco, New York, NY

Anaerobic digestion (AD) is a natural process where natural bacteria decompose organic waste in the absence of oxygen to produce biogas (a renewable fuel) and digestate (an organic soil fertilizer, amendment, or additive). Recycling excess organic-waste, creating renewable energy, and returning nutrients and carbon back to the soil all have significant impacts on reducing greenhouse gas (GHG) emissions, making AD an essential tool in reversing the effects of climate change.

Biogas is a carbon-neutral fuel, specifically when it originates from organic sources that consumed carbon dioxide (CO<sub>2</sub>) from the atmosphere during photosynthesis. When organic-waste is additionally diverted from landfills, then biogas is carbon-negative, which means that it is reducing net carbon dioxide concentrations in the atmosphere.

Biogas can be used to power boilers or generate electricity, reducing a municipality's, a company's, or campus' reliance on fossil fuels, and improving the resiliency of its energy system. Biogas can also be refined into renewable natural gas (RNG), which is fully interchangeable with conventional, fossil fuel-based natural gas. Emissions from fossil fuels, in 2017, were responsible for 76% of the total US anthropogenic GHG emissions<sup>1</sup>. Moreover, the transportation sector alone, from road travel to flights and shipping, accounts for about 23% of global energy-related CO<sub>2</sub> emissions. More specifically, fossil-based natural gas is the second major energy fuel type contributor in terms of CO<sub>2</sub> emissions into the atmosphere, 1,625 million metric tons<sup>1</sup>. Renewable natural gas can contribute to GHG emissions reduction in the transportation sector, and it is the only green alternative option for utility companies to reduce their greenhouse gas impact.

This study focuses on an organic-waste AD plant that diverts 132,000 US tons of waste from landfills and produces 275,000 MMBtu of RNG annually, which is equivalent to the electricity supply of more than 6,635 number of US-houses per year. Results show that more than 26,225 US tons of CO2eq can be saved annually, which is the same environmental impact that a US forest area 40 times the size of Central Park can provide.

### USING WASTE CARBON FEEDSTOCKS TO PRODUCE CHEMICALS.

### Elizabeth Nesbitt

Office of Industries, U.S. International Trade Commission, Washington, DC

Emerging carbon capture utilization (CCU) technologies potentially allow chemical companies and other manufacturers to capture waste carbon—in the form of carbon monoxide (CO) and/or carbon dioxide (CO2)—from industrial emissions and process it into sustainable, value-added biofuels and chemicals. Using CCU technologies to consume waste feedstocks can cut production costs; benefit the environment; monetize industrial emissions; and, depending on the region, allow companies to meet CO2 emissions goals. Moreover, using waste carbon to make chemicals can also reduce manufacturers' reliance on fossil fuels such as crude petroleum and natural gas, an important factor, particularly for the European Union and China, given the volatility in sourcing and pricing of fossil fuels, especially those that are imported.

This working paper: 1) explains carbon's critical role in the production of chemicals and as a target for industrial emissions reduction; 2) describes new CCU technologies stemming from advances in fields such as industrial biotechnology and electrolysis; 3) identifies sectors and geographical locales in which these technologies are being adopted, as well as factors driving adoption; and 4) examines potential implications for U.S. and global industrial competitiveness within one sector with high emissions, the steel industry. This paper concludes that these CCU technologies are promoting a paradigm shift that has the potential to increase firm-level competitiveness for manufacturers that adopt these processes, while also reducing the environmental impact of these manufacturers. To the extent that these technologies become widely adopted, they could result in substantial increases in supply of such chemicals globally, with potential disruptive impacts on trade and prices.

### INTEGRATION OF DIRECT AIR CAPTURE SYSTEM WITH ADVANCED PHOTOBIOREACTOR FOR SUSTAINABLE ALGAE-BASED BIOFUEL PRODUCTION.

Eric C. D. Tan<sup>1</sup>, **Kylee Harris**<sup>1</sup>, Miles Sakwa-Novak<sup>2</sup>, Yanhui Yuan<sup>2</sup>, Eric W. Ping<sup>2</sup>, Ronald R. Chance<sup>2</sup>, Valerie Thomas<sup>3</sup>, Jaden T. Johnston<sup>3</sup>, and Shavonn D'Souza<sup>3</sup> (1)National Renewable Energy Laboratory, Golden, CO, (2)Global Thermostat, Denver, CO, (3)Georgia Institute of Technology, Atlanta, GA

The continuous increase in global carbon dioxide (CO<sub>2</sub>) concentration since the First Industrial Revolution correlates convincingly with the ongoing rise of the Earth's surface temperature (combined land and ocean) that plays a critical role in extreme weather. Technologies have been developed to cut anthropogenic CO<sub>2</sub> emissions. For example, carbon capture and storage (CCS) technology is deployed to mitigate the CO<sub>2</sub> emission from large stationary point sources, such as power plants, petroleum refineries, gas processing facilities, and cement factories. CCS captured CO<sub>2</sub> is typically buried in geological formations underground for long term storage. Other transformative carbon removal technologies have also emerged, including the direct air capture (DAC) approach. DAC technologies, by definition, only capture CO<sub>2</sub> from atmosphere air, and as opposed to CCS, they do not include point source capture. If employed for biofuel production, DAC can enable the decarbonization of the transportation sector and ease the renewable feedstock competition for biofuel production. This study illustrates the integration of a DAC system with an advanced photobioreactor for sustainable algae-based biofuel production. We perform techno-economic analysis to assess economic feasibility and identify key cost drivers and life cycle assessment to quantify the supply chain greenhouse gas emissions.

DECARBONIZATION USING A COMPREHENSIVE ONE-STOP-SHOP MODEL FOR CITIES.

Ravi Malhotra

ICAST, Denver, CO

ICAST (International Center for Appropriate and Sustainable Technology) is a national 501(c)(3) nonprofit launched in 2002 to implement energy efficiency (EE) and decarbonization solutions in affordable multifamily housing (MFAH) properties. ICAST currently implements EE retrofit projects in MFAH properties in cities across the country, including nine utility EE programs in Southern California, Missouri, New Mexico, Kansas City, Utah, and Arizona. To date, 505562 tons of carbon emissions have been reduced over the lifetime of EE upgrades made by ICAST. ICAST is headquartered in Denver, Colorado.

ICAST exclusively serves multifamily (MF) properties, 90% of which are MFAH. ICAST is a national pioneer in the comprehensive "one-stop-shop" (OSS) approach, which includes energy assessments, design and engineering, construction management, access to financing, workforce training, tenant education, and reporting. ICAST employs a whole building deep energy retrofit model to deliver its OSS services, with the early retirement of inefficient systems and coverage of the entire MFAH property (in-unit residential and common area commercial meters). ICAST's OSS approach is designed to overcome the hurdles of implementing green upgrades for the hard-to-serve MFAH market. ICAST focuses on benefits beyond utility cost savings, such as increased property value, lower operating and maintenance (O&M) costs, higher occupancy levels, and lower turnover rates, which lead to higher profits for the owner. Our EE services help preserve affordable housing by improving the quality of the properties, lowering tenant utility bills, and improving the health and well-being of its low-income (LI) residents.

The benefits of the ICAST OSS approach go far beyond energy savings and utility bill savings. ICAST collects data through its M&V processes to report on economic, environmental and social impacts resulting from the upgrade including, but not limited to: carbon and GHG reductions, water savings, utility cost saving, the number of jobs created/retained, money invested into the community, number of LI residents served, and the number of disadvantaged residents provided training through the GC<sup>2</sup> workforce development initiative including the number of trainees placed in jobs.

### **RENEWABLE/ALTERNATIVE ENERGY**

### **RENEWABLE ENERGY RESEARCH SUPPORTING CALIFORNIA GOALS TOWARDS A ZERO-CARBON ELECTRICITY** AND ECONOMY.

#### Silvia Palma-Rojas

Energy Research and Development Division, California Energy Commission, Sacramento, CA

California is leading the United States towards a 100 percent clean energy future. In 2018, the State established a landmark policy requiring 60% renewable energy by 2030 and 100% zero-carbon electricity by 2045. The policy requires the transition to a zero-carbon electric system does not cause or contribute to increases of greenhouse gas emissions elsewhere in the western electricity grid.

The California Energy Commission (CEC) plays a pivotal role by developing and mandating programs that use renewable energy, incentives for energy technology installation, and provides grants for innovation, and by ensuring the efforts benefit all Californians. The CEC's research, development and demonstration programs provide more than \$200 million each year to accelerate new scientific and technology solutions that will result in a cleaner, safer, more affordable, and more resilient energy system. This paper aims to discuss some of the cutting-edge renewable energy technologies being funded by CEC and making cost and technological breakthroughs of renewable energy generation. The CEC's Research Division programs have awarded more than 87 research projects focused on advancing renewable energy generation science and technologies since 2014, providing more than \$146 million up to date. For instance, some of the solar projects have been addressing technical challenges and lab demonstrating emerging PV technologies, such as perovskite, organic, and tandem cells, as well as field testing and validating solar PV tracking solutions. Wind energy projects are advancing in materials science and applying three-dimensional concrete printing approaches to manufacture concrete towers for larger wind energy turbines. Geothermal projects are developing cost-effective approaches to recover lithium from geothermal brines and developing imaging subsurface flow paths in operating geothermal reservoirs.

The CEC research renewable portfolio is committed to decarbonize the electricity sector in an inclusive, safe, and reliable manner that includes solutions for all communities, including disadvantaged and low-income communities.

#### IONOMERS FROM KRAFT LIGNIN FOR ENERGY CONVERSION AND STORAGE DEVICES.

#### Shudipto K. Dishari

Chemical and Biomolecular Engineering, University of Nebraska-Lincoln, Lincoln, NE

Lignocellulosic biorefineries and pulp and paper industries produce lignin-rich waste (>70 million ton/yr) only a small fraction of which is utilized to produce value-added products. Innovative lignin valorization efforts are thus needed to boost bioeconomy. Also to aid in the energy economy, we need to address the major challenges on the way of large-scale commercialization of energy conversion and storage devices (such as fuel cells, redox flow batteries, and electrolyzers). A few of such challenges are reducing the cost and using environment-friendly materials for these technologies. One of the major cost components of fuel cells and batteries is an ion-conducting polymer (or ionomer). Ionomers are used in these devices as a bulk membrane separator (several tens of micron thick) and a thin catalyst binder layer (sub-micron thick) at electrode interface to promote proton conduction from anode to cathode and make the oxygen reduction reaction (ORR) efficient. The current state-of-the-art ionomer Nafion used for this purpose has multiple issues. Being fluorocarbon-based, Nafion is not environment-friendly. Also, Nafion is very expensive. Most importantly, Nafion experiences ion conduction limitations within the sub-micron thick catalyst binder layer, which negatively impacts the ORR efficiency and fuel cell performance. If the naturally abundant and waste lignin can be utilized to produce efficient proton conducting materials, the environment can be preserved, the cost of renewable energy-driven technologies can be significantly minimized with improved performance. As a continued effort along this direction, this work focused on designing ionomers from kraft lignin (LS) using sulfomethylation reaction. Unlike commercial lignosulfonate, our ionomers with suitable ion exchange capacities (IECs) were not water soluble. Therefore, these ionomers were ideal for water-mediated ion conduction for practical energy applications. LS showed great promise as catalyst binder for fuel cell electrodes since the ion conductivity of LS was significantly higher than Nafion in sub-micron thick films. The thin film morphology, water uptake, and hydration induced changes in ionic domain characteristics of LS films were systematically explored and compared with Nafion to understand the route to the efficient ion conduction of LS ionomers. This work can inform and guide the future design of lignin-based ionomers.

### ON-DEMAND RELEASE OF HYDROGEN FROM COPPER-LOADED COVALENT ORGANIC FRAMEWORKS THROUGH PHOTODISSOCIATION.

### **Wade Braunecker**<sup>1</sup>, Rachel Mow<sup>1,2</sup>, Sarah Shulda<sup>1</sup>, Kurt Van Allsburg<sup>3</sup>, Gabriella Lahti<sup>3</sup>, Derek Vardon<sup>3</sup>, and Thomas Gennett<sup>1,2</sup>

(1)Chemistry and Nanoscience Center, National Renewable Energy Laboratory, Golden, CO, (2)Colorado School of Mines, Golden, CO, (3)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO

Successful strategies for tuning H<sub>2</sub> binding enthalpies that could be broadly applied to solid state sorbent materials would have profound implications on the overall viability of large-scale H<sub>2</sub> storage and delivery. Here, we demonstrate that copper(II) formate can be efficiently incorporated into the pores of 2D and 3D imine-based covalent organic frameworks (COFs) via coordination with Schiff-base ligands in the COF. The coordinated Cu(II) can then be reduced to Cu(I) with a thermal treatment that evolves CO<sub>2</sub> and produces an open metal binding site. Remarkably, upon loading with H<sub>2</sub> gas, the activated Cu(I) COF retains adsorbed H<sub>2</sub> above room temperature. Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) measurements support a molecular hydrogen-type interaction with Cu(I). The material can be cycled > 40 times without loss in H<sub>2</sub> storage capacity. Furthermore, using temperature programmed desorption measurements, we demonstrate how long-wave ultraviolet light can be used to efficiently desorb H<sub>2</sub> over a range of temperatures. We discuss these results in the context of other recent literature work on the photodissociation of small molecules from Cu(I) complexes where light induces a metal-to-ligand charge transfer that influences small molecule and gas binding enthalpies.

The results represent an advance toward 'on-demand' delivery of H<sub>2</sub> in a highly stable and versatile material.

### NUTRIENT POLLUTION, PREVENTION, AND CONTROL

#### EPA'S SCIENCE TO SUPPORT NUTRIENT-RELATED WATER QUALITY GOALS.

#### Anne Rea

#### ORD, EPA, Research Triangle Park, NC

Nutrient pollution is the most widespread water quality problem facing the United States, with far-ranging consequences for environmental condition, economic prosperity, and human health and well-being. The U.S. Environmental Protection Agency's (EPA) Nutrients and Harmful Algal Blooms research is housed within the Office of Research and Development's (ORD) Safe and Sustainable Water Resources Research Program (SSWR). It supports EPA's Office of Water (OW), which has specific research needs as it develops new tools for states, tribes, and local decision-makers to establish and achieve water quality goals. ORD's research under SSWR includes laboratory analyses, monitoring, modeling, and decision-support approaches to inform the protection of different types of waters (e.g., streams, lakes) for different designated uses (e.g., aquatic life, recreation, and drinking water source protection). Establishing nutrient-related water quality management goals requires an understanding of the impacts of excess nutrients on water bodies and aquatic life, and the processes affecting their recovery.

An overview of nutrients research in EPA ORD will be provided, focusing on studies that support the key OW objective of attaining nutrient-related water quality goals. This presentation will summarize research that 1) provides information, methods, or approaches to determine nutrient-related impacts in watersheds and water bodies, 2) relates the condition of watersheds and water bodies to nutrient loading, water quality, and aquatic life; and 3) integrates these results to identify effective approaches for restoration and recovery. This research advances the science needed to inform decisions related to nutrient water quality goals of EPA program offices, EPA regions, states, and tribes.

### NUTRIENT POLLUTION MANAGEMENT BY COORDINATION NETWORKS AND RECOVERY TECHNOLOGIES CONSIDERING ENVIRONMENTAL GEOGRAPHIC INFORMATION.

Gerardo J. Ruiz-Mercado<sup>1</sup>, Mariano Martín<sup>2</sup>, and Victor M. Zavala<sup>3</sup>

(1)Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH, (2)Department of Chemical Engineering, University of Salamanca, Salamanca, Spain, (3)Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

The uncontrolled release of nutrients (e.g. phosphates) into the environment from anthropogenic activities such as livestock management triggers eutrophication, harmful algal blooms (HABs), and other undesired ecosystem responses. Particularly, HABs pose severe health threats and ecological impairments due to the release of toxins and the appearance of hypoxia in water bodies, and economic losses since they affect tourism, recreational and commercial activities.

Therefore, it is necessary to ease more efficient time-location nutrient source management actions and programs to aid in reducing nutrient pollution, and subsequent effects on watersheds and waterbodies.

This contribution describes a multi-scale framework for the prevention and control of nutrient pollution and ecosystem responses (e.g., HABs) by implementing on-site nutrient recovery technologies and coordination network strategies.

The first framework part aids in the evaluation and selection of the most suitable nutrient recovery technology for livestock facilities. It is based on geospatial environmental sensitivity to nutrient pollution caused by legacy and new inputs of nutrients at watershed resolution. Also, the framework can provide a customized cost-effective solution for individual livestock facilities by evaluating different state-of-the-art nutrient recovery technologies together with power and biofuels generation as an additional source of revenue.

The second framework part incorporates a coordination network strategy to identify optimal locations for nutrientrich waste (manure) storage and transportation, nutrient and energy recovery technology evaluation for revenue generation, a nutrient transport model which captures time and location of nutrient flow from agricultural lands to water bodies, and assesses nutrient impact ecosystem responses across scale (e.g., HABs).

This framework has the potential to be a key asset for state and regional partners to develop nutrient pollution and ecosystem integrated responses at regional spatial resolution.

### QUANTIFYING VIRTUAL P INPUTS TO AGRICULTURAL COMMODITIES INCLUDING CORN ETHANOL.

### Mikaela Algren<sup>1</sup>, Christine Costello<sup>2</sup>, and Amy E. Landis<sup>1</sup>

(1)Civil and Environmental Engineering, Colorado School of Mines, Golden, CO, (2)Agricultural and Biological Engineering, The Pennsylvania State University, University Park, PA

Phosphorus (P) uses in agriculture are extremely inefficient. Globally, around half of the P applied as fertilizer is lost from fields into waterbodies. This P contributes to eutrophication which can lead to algal blooms, hypoxia, and fish kills, especially in inland lakes and waterbodies. Losses of P from the economy are also problematic because P is an essential and finite resource with no known substitute, and future P resources must meet the rising food and energy needs of an increasingly affluent and growing world population. The P inputs to land required for production of specific commodity agricultural products, including corn ethanol, are not well understood. Therefore, the Net Anthropogenic Phosphorus Inputs (NAPI) toolbox has been modified to create a commodity-specific P inputs model (CSNAPI) for quantifying the P inputs required to produce 16 commodity crops (corn, soy, wheat, etc.), ethanol fuel, ethanol coproducts, and 9 animal food products (beef, milk, pork, etc.) in the United States. The model includes commodity-specific estimates of P fertilizer inputs for all products and P diet-supplementation for animal food products. In this presentation, we present CSNAPI results quantifying the P inputs to US agricultural commodities and compare these results to those published in previous studies.

### FOOD, ENERGY, WATER NEXUS

#### BLACK SWAN CYCLE FOR ENERGY CARBON MANAGEMENT.

#### Brian Kolodji

CEO, Black Swan, LLC, Bakersfield, CA

The Black Swan Cycle is a suite of energy carbon management technologies that uses proven gas processing innovations to reduce power plant fuel consumption in a "plug and play" manner for existing systems by up to 50% without impacting power generation duty. Conditioned flue gas saves additional fuel with heat and waste heat recovery systems. The flue gas is then capable of being readily applied using decades proven crop carbon enrichment practices to increase agricultural yield by up to 100% and water utilization efficiency by 20% to bring return on investment under two years. Results from four pilot plants and a demonstration facility across from a California refinery funded by the California Department of Food and Agriculture will be presented.

### A MULTI-OBJECTIVE OPTIMIZATION MODEL TO PLAN CITY-SCALE WATER SYSTEMS WITH ECONOMIC AND ENVIRONMENTAL OBJECTIVES: A CASE STUDY IN SANTIAGO, CHILE.

**Daniela Gormaz-Cuevas**<sup>1</sup>, Javiera Riffo-Rivas<sup>1</sup>, Ludovic Montastruc<sup>2</sup>, and Felipe Díaz-Alvarado<sup>1</sup> (1)Departamento de Ingeniería Química, Biotecnología y Materiales, Universidad de Chile, Santiago, Chile, (2)Laboratoire de Génie Chimique (LGC), Université de Toulouse, Toulouse, France

Climate Change and its effects in water scarcity has become an important challenge for cities with water management problems. These problems require an integral planning of the city, which can be supported by optimization, so the main objective of the research is to provide a regional optimization model for water networks, implemented in a case study. The model is formulated as a multi-objective mixed-integer programming problem, focused on environmental and economic impact of the network, minimizing water extracted from natural sources and total cost. The model cover a complete existing city-scale water network, including 4 different options of water reuse within the city: drinking water, fresh water, irrigation, and discharge in natural courses. The case study is Santiago, capital of Chile, which is the political, economic, and institutional center of Chile. The results show the installation of a new drinking water treatment plant (DWTP) and a new waste water treatment plant (WWTP) with drinking output quality. The optimal solution also shows the modification of the two existing waste water treatment plant, with drinking and irrigation output quality each one. The results allow a reuse of water within the network, and also indicate that it is more environmentally and economically convenient to reuse for irrigation and drinking water consumption rather than other options. The model can be implemented in other contexts, allowing better planning of water resources in any city.

### **Short Presentations**

### **30 YEARS OF SOFT INTERVENTIONS TO REDUCE CAR USE - A SYSTEMATIC REVIEW AND META-ANALYSIS.**

#### Alin Semenescu

### Department of Psychology, West University of Timișoara, Timișoara, Romania

Soft interventions are generally regarded as effective means for reducing personal car use. However, some authors have raised doubts about the validity of such claims. These doubts are fueled primarily by the low methodological quality of evaluation studies upon which such conclusions are based and by the fact that the literature is, for the most part, narratively synthesized. The present systematic review addresses these issues by investigating the effect of soft interventions on car use through a meta-analysis, which includes only experimental and well-controlled quasi-experimental studies. Results revealed that interventions (k = 45) lead to a significant reduction of 7% in car modal split share (Hedges' g = .170). Moderators of interventions and by the main *psychological variable targeted* by the interventions. The other studied moderators (i.e. *residential relocation* of participants, *study design, percentage of females* in the study, the presence of *incentives*, passed *time to follow-up*, interventions' *measurement instrument*, *city size* in which interventions were applied and the *setting* where they were conducted) were non-significant. Limitations of the present findings, together with implications for policy and practice are discussed.

### TOWARD CARBON NEUTRAL INDUSTRIAL PARK DESIGN USING RESOURCE INTEGRATION.

### Farah Ramadan, Taha Kubbar, and Elizabeth Abraham

Chemical Engineering, Texas A&M University at Qatar, Doha, Qatar

In response to climate change concerns, there has been an increasing global need to reduce carbon dioxide emissions. These emissions are largely due to stationary industrial processes, which are typically concentrated in industrial parks. In recent years, there has been an increased focus on carbon capture utilization and storage (CCUS) solutions. Many approaches have been developed to integrated resources such as natural gas, energy, and carbon dioxide to design industrial parks systematically. However, these approaches mostly looked at a separate resource at a time. This work aims to find a sustainable solution to continue the production of many chemical products while ensuring overall profitable production with zero carbon footprint. This is done by using an optimization model<sup>1</sup> that integrates the plants and incorporates energy reuse to maximize the profit. The integration approach will produce value-added products from natural gas, water, air, emissions, and energy (as heat and power) in a carbon-neutral industrial park. The approach considers plants that fulfill the three selection criteria: commercialization, integration with other plants, and return on investment. The approach uses a Linear Program (LP) to screen all possible plant combinations and determine the optimum configuration for a set objective. A sensitivity analysis is then performed on the process parameters. This method demonstrated through an example that includes processes that either convert hydrocarbons, can produce or consume carbon dioxide and explores the effect of renewable energy use. The objective is set up to design a carbon-neutral industrial park using the selected processes that would achieve maximum profitability. The results demonstrated that the integration of these processes was able to achieve profitability based on the price and source of energy. The model was thus able to show that process integration, mainly through the integration of multiple resources, is a means to produce value-added products that can minimize an industrial city's carbon footprint effectively.

### BEAD ACTIVATED CARBON IN A FLUIDIZED BED CONCENTRATOR CONTROLS EMISSIONS & RECOVERS TERPENES FROM DRYING WOOD.

### Kim Tutin

Chemicals, Georgia-Pacific, Decatur, GA

**Problem:** The industry standard control device to reduce organic carbon emissions, the Regenerative Thermal Oxidizer (RTO), controls emissions by oxidation (incineration) of organic carbon emissions to carbon dioxide (CO2). The typical RTO has an annualized cost of \$8-\$33 per standard cubic feet per minute (sCFM)<sup>1</sup> and creates CO2 emissions<sup>2</sup> commonly referred to as greenhouse gas (GHG) emissions. Operating expenses are due to natural gas usage, electricity usage, media replacement costs, and maintenance costs.

**Potential Solution:** An alternative emissions control system to reduce lifetime costs and avoid greenhouse gases from oxidation uses Bead Activated Carbon (BAC) in a Fluidized Bed Concentrator (FBC) to adsorb emissions. Compared to the industry standard Oxidation system, the FBC utilizes less energy, creates less GHG, and avoids oxides of nitrogen (NOx) emissions from combustion that are an undesirable precursor to secondary formation of ozone and fine particulate matter.<sup>3</sup> This project demonstrates the feasibility of sustainably using an FBC to control (adsorb) emissions and recover terpenes from commercial wood drying operations such as those utilized in the manufacture of engineered wood products e.g. Oriented Strand Board (OSB), plywood, and particleboard and wood pellets. The FBC technology could be used at over 50 potential sites for emissions control.

**Scope:** The scope of this project is the technology's use in a wood drying application. However, the technology is currently in use for emissions control in a broad variety of applications including painting, electronics manufacturing, and chemical manufacturing.<sup>6</sup>

**SUMMARY:** Key findings from the project indicate that:

- Environmental personnel are supportive of permitting for commercial FBC system. This input was received from one expert at the Environmental Protection Agency (EPA), from personnel at two state agencies (each state will be different), and from environmental personnel internal to Georgia-Pacific.
- Modeling of energy required to operate the FBC was reduced as compared to the industry standard RTO. Energy reductions translate to both operational cost savings and GHG emissions reductions for the FBC as compared to the industry standard, the RTO.
- FBC system recovered terpenes as a valuable bioproduct.
- Next step is to scale up to an industrial FBC system and commercialize the technology.

### DECARBONIZATION OF SHALE GAS USING DEEP EUTECTIC SOLVENTS.

### **Pranjal Maheshwari**, Mohd Belal Haider, and Rakesh Kumar Chemical engineering, Rajiv Gandhi Institute Of Petroleum Technology, AMETHI, India

The drastic change in climatic conditions is a major challenge faced by society. Secure, affordable and reliable energy supplies are essential for economic growth, but increases in the CO<sub>2</sub> emissions are the cause of major concern. Carbon capture and storage (CCS) involves the capture of CO<sub>2</sub> from the emissions generated mainly due to combustion of coal or natural gas and includes the further sequestration of the captured CO<sub>2</sub> in the particular geological formations. Recently, Deep Eutectic Solvents (DESs) similar to that of lonic Liquids have shown the ability to capture CO<sub>2</sub>. They comprise of salt and another compound as hydrogen bond donor (HBD) resulting in a low melting point mixture. DESs usually have low melting temperatures due to the formation of their intermolecular hydrogen bonds. Charge delocalization in DESs is the main reason behind the low melting points then of the individual constituents. The Hydrogen bonds play a significant role in the more effective binding of CO<sub>2</sub> molecules by DESs compared to that of classical ILs. Present work focuses on modelling and simulation of CO<sub>2</sub> removal from Shale Gas using two effective deep eutectic solvents (DESs) reline and ethaline. The experimentally calculated solubility results of CO<sub>2</sub>, as well as methane in the reline and ethaline along with the physicochemical properties of DESs, were done for the modelling and simulation of CO<sub>2</sub> removal studies. CO<sub>2</sub> solubility experiments were carried out using Preessure Drop Method. Peng robinsson Equation of Sate was used to model the Vapor Liquid Equilibrim Data. Further, Purity of Shale Gas was compared.

### LIGNIN VALORIZATION INTO SPECIALTY CHEMICALS: SUSTAINABILITY ASSESSMENT OF AN INTEGRATED BIOREFINERY.

### **Ramsharan Pandey**, Na Wu, Ghasideh Pourhashem Coatings and Polymeric Materials, North Dakota State University, Fargo, ND

Lignin is the second most abundant biopolymer on earth. Technical lignin is primarily produced by paper and pulp industries while second-generation biorefineries are the prospective producers. Currently, the bulk of lignin produced is burned as a low-value fuel. The economic feasibility of a biorefinery producing biofuel is still lacking due to the higher cost of biofuel. Valorizing lignin into specialty chemicals can provide biorefinery with additional revenue and lower the price of biofuel. Lignin valorization can be achieved through multiple possible pathways including depolymerization, chemical modification, and macromolecular application. Potential application areas of lignin include aromatic chemicals, binders, adhesives, additives for different applications like food and concrete, carbon products like carbon fiber and activated carbon, and polyurethane foams. Macromolecular lignin applications can be achieved through direct application of lignin in the desired process, or chemically modifying lignin to achieve higher reactivity of lignin as well as improved properties. But there is yet a dearth of economic and environmental analyses of macromolecular lignin applications to further inform the steps required for their future commercialization. In this study, we will investigate the feasibility of valorizing lignin into specialty chemicals like resins, in an integrated biorefinery setup. We examine the scaled-up process of chemically modifying by-product lignin stream in a biorefinery into acetoacetylated lignin resin through process modeling and look into the economicenvironmental performance of the integrated biorefinery as a whole. We use techno-economic analysis (TEA) to determine the major utilities and capital costs and suggest areas that need to be optimized for higher economic profitability. Additionally, we use the Life cycle assessment (LCA) method to assess the environmental impacts of coproducing biofuels and lignin-based polymers. The results from this study can be valuable in realizing the potential of lignin in integrated biorefinery setup and provide direction for future research work.

### **RECYCLING COCONUT HUSK FIBRE IN PAVING MATERIAL AS AN ENVIRONMENTALLY ATTRACTIVE WASTE SOLUTION AND ASPHALT MODIFIER.**

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Trinidad and Tobago (T&T) is a Small Island Developing State has embarked on economic diversification away from oil and gas and the development of a sustainable economy fostering growth in the manufacturing, agriculture and service sectors. Through the introduction of the National Environmental policy, the country has emphasized waste management and environmental conservation strategies geared towards creating employment opportunities and business development. The disposal of waste coconut husk (WCH) is either via dumping in landfills or via illegal dumping in waterways and at the side of roadways, both having negative health and environmental effects. The reuse of WCH as an additive for road paving applications has been a successful mitigation strategy in foreign jurisdictions, however there is a lack of required scientific data such as the optimum dosages and fibre length required for use with indigenous asphaltic binders for the implementation of the strategy locally. To fill this information gap, this study investigated the influence of WCH on the rheological properties of Trinidad Lake Asphalt (TLA) and Trinidad Petroleum Bitumen (TPB). The rheological properties of complex modulus (G\*) and phase angle ( $\delta$ ), fatigue cracking resistance ( $G^*sin\delta$ ) and rutting resistance parameters ( $G^*/sin\delta$ ) of mixes with WCH of lengths 2.5mm and 5mm and dosages (up to 8% wt.) were measured. The study showed that the modified blends containing 4% WCH in TLA and 2% WCH in TPB of fibre lengths 2.5 mm resulted in the best rheological performances with the highest G<sup>\*</sup> and lowest  $\delta$  values. These blends also exhibited the best fatigue cracking resistance and rutting resistance characteristics evidenced by the lowest values of  $G^*sin\delta$  and highest  $G^*/sin\delta$ , respectively. This study proved that the strategy of incorporating WCH into TLA and TPB is a sustainable strategy for WHC disposal while also providing an added benefit of enhancing the performance characteristics of the asphaltic binders and provides the lacking scientific data required for the implementation of this strategy in TT.

### A DESIGN AND FEASIBILITY STUDY OF AN ACTIVATED CARBON PRODUCTION FACILITY IN TRINIDAD AND TOBAGO.

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Trinidad and Tobago (TT) is a highly industrialized oil and gas-based economy; however, within recent times, the focus has shifted towards economic diversification guided by sustainable development strategies as outlined in the Vision 2030 National Development Policy. In pursuit of one of the sustainable development goals of waste reduction by improved waste management and recycling systems, the issue of the indiscriminate disposal of waste coconut shells, a by-product of the robust coconut industry, is receiving national attention. Its widespread, indiscriminate disposal is associated with negative environmental impacts such as flooding and a breeding ground for rodents and mosquitos. Research has shown that many countries have successfully converted waste coconut shells into activated carbon (AC), thus not only producing a useful and valuable product but also providing a sustainable strategy for the disposal of the waste material. In TT, AC is utilized in water and wastewater treatment and food manufacturing sectors. AC is currently imported at high costs using scarce USD foreign exchange, and the abundantly available coconut shell locally and regionally suggests that an activated carbon production facility in TT has immense potential. To implement such a strategy locally, there is a need for data relating to the design and evaluation of an activated carbon manufacturing plant to meet local needs, and this information gap forms the basis of this study. The optimum design obtained involves the primary process of carbonization of the coconut shells at 600°C for 150 mins, followed by steam-activation of the char at 900°C for 60 mins. An economic evaluation of this facility with a production capacity of 1225 tons/year to meet local needs was found to be feasible, with an associated Net Present Value (NPV) of USD 17,747,598, an Internal Rate of Return (IRR) of 23.1% and a Payback Period of 4 years. TT's substantial supply of natural gas further supports this biomass conversion initiative, the benefits of which include the supply of activated carbon both locally and regionally, allowing for diversification of the economy, increased employment opportunities, and an innovative solution to the end-of-life challenges faced within the local coconut industry.

### REUSE POTENTIAL OF SPENT MEDIA FILTER AS AN ADDITIVE FOR TRINIDAD ROAD PAVING APPLICATIONS.

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Trinidad and Tobago (TT) is a highly industrialized country in the Caribbean. Its economy boasts of a vibrant manufacturing sector producing commodities such as petrochemicals, construction materials and food and beverage products. TT, through the creation of the National Environment Policy, is committed to the enhancement of recovery, recycling and reuse of waste material, providing alternative avenues for waste disposal and creating economic activity. The edible oil industry produces spent media filter (SMF) accumulated during the bleaching stage of the manufacturing process. SMF has negative environmental and health impacts and is currently dumped in landfills. The possibility of reusing SMF as an additive to enhance the performance of road paving materials in TT namely Trinidad Lake Asphalt (TLA) and Trinidad Petroleum Bitumen (TPB) was evaluated by studying the influence of the SMF on the rheological properties of complex modulus (G<sup>\*</sup>), phase angle ( $\delta$ ), viscosity, rutting resistance (G<sup>\*</sup>sin  $\delta$ ) and fatigue cracking resistance (G<sup>\*</sup>sin  $\delta$ ).

Optimum dosages of SMF resulting in maximum stiffness and elasticity ((high G\* and low  $\delta$  respectively), as well as viscosity, were 1% and 2% for TLA and TPB, respectively. Compared to the unmodified TLA material, improvement in the rutting resistance was observed with the 1% SMF addition while the fatigue cracking improved with the 1% and 8% SMF addition for TLA. For TPB, improvements were noted with 1% SMF addition for fatigue cracking and 2% SMF addition for rutting resistance. These results were confirmed by the shapes of the black curves obtained for each material. Optimum dosages observed for fatigue cracking and rutting resistance for TLA and TPB also demonstrated superior temperature susceptibility characteristics. The results of this study offer evidence that the addition of SMF to asphaltic materials used in road paving in TT can enhanced performance characteristics of the modified blends while also serving as a reuse strategy to mitigate the disposal issues associated with SMF. This study provides the basis for future work towards the implementation of this strategy.

### UNDERSTANDING THE EFFECT OF SURFACE CHARACTERISTICS ON ATTACHED GROWTH OF TURF-FORMING FILAMENTOUS ALGAE.

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This research aims to understand the effect of surface energy and topography of the attachment substrate on the attached growth of turf-forming filamentous algae Stigeoclonium. A subcategory of attached algal cultivation systems, Algal Turf Scrubbers (ATS), are often dominated by turf forming filamentous algae. These systems are known to be effective in removing excess nutrients such as nitrates and phosphates from water coupled with algal biomass production. Algal biomass is a source of valuable bio-compounds and has potential applications in industries such as biofuels, pharmaceuticals, cosmetics, animal feed, human food, fertilizer, industrial enzymes, and bioplastics production. Right now, yield consistency and cost efficiency are among the major challenges in the commercialization of algae-based products and processes. Attached algal cultivation systems, including ATS systems, are a less explored group of algal cultivation systems with substantial potential for environmental remediation and improving the cost and energy efficiency of algal biomass production. However, limited fundamental scientific understanding of the algal attachment process hinders the ability to optimize algal attachment and growth. This especially true for turf-forming filamentous species. In this research, substrates with different surface energies were used to cultivate filamentous algae Stigeoclonium in a flow reactor, and the amount of attached biomass was measured. Furthermore, 3D printed polylactic acid substrata with macroscopic spherical topographical features were investigated for attachment favorability. Results from this study show the correlation of early-stage colonization with surface energy and the effect of macroscale topographical features of the surface on the biomass cultivation.

### A STUDY ON THE QUALITATIVE CHARACTERISTICS OF VARIOUS LIGNIN FRACTIONS ISOLATED FROM PINEWOOD BIOMASS VIA AN ORGANOSOLV PROCESS.

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Lignocelluloses are the most abundent and readily collectable biomass feedstcoks on this earth and even more with an enough theoratical potential to replace existing fossilfuels based economy. In their typical nature configuration, they are composed of polysaccharides as well as lignin. This lignin is the second most abundant component in their structure and is often a biorefinery waste in a typical 2G bioethanol production schemes. This lignin, actually, is a rich diverse feedstock for the production of various composites, sustainable materials, epoxies and even can be used in medicine and for drug delivery. For this lignin to be isolated with as much little modification as possible is still a challenge for the establishment of lignin-first 2G biorefineries. Therefore, we are trying to adapt and develop such processes that are able to extract/ isolate lignin from the native structure with least and/or no modification. We are applying several organsolv fractionation processes like a green solvent gamma valerolactone (GVL), ethanol, combination of ethanol, GVL and the synergetic effects of GVL, ethanol under mild acidic and thermal conditions. We have used mild temperature conditions ranging from 50 °C to 90 °C and time ranges from 3 hrs to 6 hrs. In order to induce mild acidic conditions Hcl was employed as a catalyst with few drops only. The lignin fractions separated via this method are subjected to their qualitative analyses such as (Defunctionalization Followed by Random Carbonization) DFRC, Gel permeation chromatography (GPC) and their FTIR analyses to further sort out any clue with their effect on lignin purity and yield. All the obtained results are studied as a comparison with the classical protolignin i-e Milled Wood Lignin (MWL).

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