NASCRE-5 Oral Presentation Program

Sunday, Feb 16: Workshops (11:30-16:30) and Welcome Reception (18:00-19:30)

Day 1: Monday, February 17				
8:15-9:15 AM	Plenary 1: Developing Strategies for Polymer Redesign and Recycling Using Reaction Pathway Analysis ***Linda Broadbelt*** *(Northwestern University)*			
9:15-9:30 AM	Refreshment Break			
9:30-10:30 AM	Plenary: Amundson Award Lecture A Personal Journey to Reaction Engineering: From Multiscale Modeling to Sustainable Processes ***Dion Vlachos*** *(University of Delaware)*			
10:30-10:45 AM	Refreshment Break			
	Room 1	Room 2	Room 3	Room 4
	Polymer Upcycling Chairs: Kim McAuley (Queens University), Michele Sarazen (Princeton)	**Fundamentals of CRE** Chairs: Hilal Ezgi Toraman (Penn State), Gregory Patience (Polytechnique Montreal)	**Reaction Engineering for the Energy Transition: 1** Chairs: Pavel Kots (NYU), Daniel Trahan (Dow)	**Novel Reactors and Process Intensification: 1** Chairs: Chris Paolucci (UVa), Dongxia Liu (U. Delaware)
10:45-11:05 AM	Revealing the Role of Mass Transfer–Chemical Kinetics Coupling in Neat and Catalytic High-Density Polyethylene Pyrolysis; *M.* ***Doga Tekbas***	Keynote: HARNESSING COUPLED REACTION-TRANSPORT PHENOMENA TO DEVELOP STABLE AND SELECTIVE ZEOLITE CATALYSTS FOR OLEFIN OLIGOMERIZATION TO TRANSPORTATION FUELS; ***Rajamani Gounder***	MODELING OF A HEAT-INTEGRATED BIOMASS DOWNDRAFT GASIFIER WITH CONSTRUCTION AND DEMOLITION WASTE AS FEEDSTOCK; ***Houda Haidar***	Microfluidic Laser-Induced Nucleation of Iron (II, III) Oxide Nanoparticle-Doped Supersaturated Aqueous KCl solutions; ***Kelechi Ndukwe-Ajala***
11:05-11:25 AM	Understanding Reaction Environments in Mechanocatalytic Processes; ***Kinga Golabek***	LENGTH EFFECTS ON PRCFD-DERIVED FIXED-BED RADIAL HEAT TRANSFER PARAMETERS; ***ANTHONY DIXON***	Radio Frequency Heating of Catalytic Propane Dehydrogenation: Finite Element Approach, Techno-Economic, and Environmental Assessment. ***Ankush Rout***	Novel modular, layered rector for continuous, scalable, efficient hydrogenation; ***Lorenzo Milani***
11:25-11:45 AM	H_2-Free Conversion of Condensation Polymers with Organic H2 Carriers - Kinetic Coupling of Hydrogenolysis and Dehydrogenation Pathways; ***Manish Shetty***	Mechanistic and Kinetic Role of Pd in the Co-Production of Ethylene and Acetic Acid from Ethane over Pd-MoV Oxides; ***Joseph Lane***	CAPITALIZING ON BIPHASIC SYSTEMS FOR THE REACTION WITH IN SITU EXTRACTION OF SUGARS TO FURANS: SOLVENT SELECTION AND REACTION MODELLING; ***Dominik Soukup-Carne***	MECHANISTIC ASPECTS OF SELECTIVE HYDROGEN COMBUSTION (SHC) OVER NA_2WO_4/SIO_2 CATALYSTS; ***Elijah Kipp***
11:45-1:15 PM	Lunch on own			
1:15-2:15 PM	Panel Discussion: 'Academia-Government-Industry: Advancing Reaction Engineering at the Interfaces Facilitator: **Nick Thornburg** (NREL) Panelists: **Jean Tom** (Princeton University), **Fabio Ribeiro** (Purdue University), **Simon Bare** (SLAC), **Triantafillos J. Mountziaris** (University of Houston)			
2:15-2:30 PM	Refreshment Break			
	Pioneers in CRE: 1	**Fundamentals of CRE** Nitish Mittal (ExxonMobil), Udit Gupta (Siemens)	**Reaction Engineering for the Energy Transition: 2** Chairs: Hsu Chiang (Oxy), Joseph Dewilde (Dow)	**Novel Reactors and Process Intensification: 2** Chairs: Rajamani Gounder (Purdue), Eric Sacia (AbbVie)

2:30-2:50 PM	Elucidating complex interactions in non-thermal plasma-assisted reactions on (supported) porous catalysts ***Michele Sarazen***	Redefining Bi-reforming of Methane at a Molecular Level Through Specific Metal-Support Interactions; *Meghana* ***Sucharita Idamakanti***	Decarbonization of Hydrogen Supply Chain via Electrification: Methane Reforming and Ammonia Decomposition ***Ram Ratnakar***	Forced Dynamic Operation of Propylene Selective Oxidation on Bismuth-Molybdate Structured Catalysts: Experiments and Modeling; ***Mohammad Moniruzzaman***
2:50-3:10 PM	Fast-Cat: A Self-Driving Catalysis Lab for Autonomous Reaction Pareto Front Mapping ***Milad Abolhasani***	A new method for the simulation of catalyst deactivation in fluidized bed reactors; ***Andrea Pappagallo***	Catalytic and Inhibitory Effects Induced by Noncovalent Interactions between Cellulose and Lignin During Fast Pyrolysis; ***Fuat Sakirler***	SELECTIVE CHEMICAL LOOPING COMBUSTION OF ACETYLENE IN ETHYLENE-RICH STREAMS; ***Matthew Jacob***
3:10-3:30 PM	Effect of Blending Hydrogen with Natural Gas on Selective Catalytic Reduction of NOx for Stationary Power Applications ***Bihter Padak***	Quantifying Reaction-Diffusion Rates of Nonoxidative Coupling of Methane per Active Edge Sites of Two-Dimensional Pt Nanolayer Catalysts; ***Tobias Misicko***	HIGHLY EFFICIENT AND STABLE IRON MOLYBDATE ELECTROCATALYST TOWARDS OXYGEN EVOLUTION REACTION UNDER ALKALINE CONDITIONS; ***FNU Vidhi***	CO_2 absorption kinetics measurements: conversion of a stirred tank to a Lewis cell; ***Jonathan Sheavly***
3:30-3:50 PM	Refreshment Break			
	Pioneers in CRE: 2	**Fundamentals of CRE** Nitish Mittal (ExxonMobil), Udit Gupta (Siemens)	**Reaction Engineering for the Energy Transition: 3** Chairs: Hsu Chiang (Oxy), Joseph Dewilde (Dow)	**Novel Reactors and Process Intensification: 3** Chairs: Fateme Rezaei (U. Miami), Onkar Manjrekar (Abbvie)
3:50-4:10 PM	Electrocatalytic Synthesis and Utilization of Nitrates for Resilient Nitrogen Circular Economy ***Meenesh Singh***	FROM PULSES TO PELLETS TO PACKED BEDS: UNDERSTANDING CrOx/Al2O3 CATALYST DEACTIVATION DURING PROPANE DEHYDROGENATION VIA TRANSIENT KINETIC ANALYSIS AND MULTISCALE MODELING; ***Nicholas Thornburg***	Experimental Analysis of a Sabatier reactor for Renewable Natural Gas Generation from Biogas: Ignition, Parameter Sensitivity Analysis, and Stability; ***Yichen Zhuang***	Applications of Countercurrent Multiphase Reactors for Maximizing Performance ***James R. Lattner***
4:10-4:30 PM	Catalytic consequences of plastic additives on bifunctional reactions of alkanes ***Gina Noh***	Polymer Distribution Models for Polyether Polyols; ***Arjun Raghuraman***	Electrification of Steam Methane Reforming by Joule Heating of Nickel-Coated High-Resistance Wires; ***Elmer Ledesma***	Overcoming the Selectivity-Conversion Tradeoff during Forced Dynamic Operation of Ethane Oxidative Dehydrogenation; ***Austin Morales***
4:30-4:50 PM	***Kate Bjorkman (Lanzajet)***	From Apparent Kinetics to Microkinetics: Leveraging Power duLaw Models for Reaction Mechanism Identification; ***Fernando Vega-Ramon***	BENCH-SCALE MULTI-TUBULAR MEMBRANE CONTACTOR REACTOR FOR FUEL PRODUCTION; ***Mohammad Bazmi***	IGNITION-EXTINCTION ANALYSIS OF OXIDATIVE DEHYDROGENATION OF ETHANE OVER M1 CATALYST IN A MONOLITH REACTOR; ***Dhagash M. Pandit***

Day 2: February 18				
8:15-9:15 AM	Plenary 2: Current Trends and Opportunities for Reaction Engineering to Impact the Pharmaceutical R&D Pipeline *Shailendra Bordawekar, AbbVie*			
9:15-9:30 AM	Refreshment Break			
9:30-10:30 AM	Plenary: Aris Award Lecture The Many Lives of Active Oxygens in the Energy Transition *Praveen Bollini (University of Houston)*			
10:30-10:45 AM	Refreshment Break			
	Room 1	Room 2	Room 3	Room 4
	Computational Chemistry and Catalysis, Data Science, ML: 1 Milad Abolhasani (NCSU), Gaurav Giri (UVa)	**Automation/Digitization in Reaction Engineering: 1** Chairs: Jake Gold (Dow), Meenesh Singh (UIC)	**Reaction Engineering for the Energy Transition: 4** Chairs: Hsi-Wu Wong (UMass Lowell), Kevin Modica (Dow)	**Novel Reactors and Process Intensification: 4** Chairs: Fateme Rezaei (U. Miami), Onkar Manjrekar (Abbvie)
10:45-11:05 AM	Using Molecular Modeling and Machine Learning to Address Stability Challenges for Zeolite Catalysts ***Chris Paolucci***	Advantages of AI-based models over mechanistic models in the dynamic optimization of fixed- and fluidized-bed reactors; ***Mauro Andrea Pappagallo***	DYNAMIC OPTIMIZATION OF ELECTRIFIED ETHANE CRACKING FOR COST-EFFECTIVE ETHYLENE PRODUCTION WITH LOW CO_2 EMISSIONS; ***Alexandre Cattry***	In-situ characterization of Ni-BaH_2 catalyst for low temperature ammonia production through chemical looping; ***Antoine Dechany***
11:05-11:25 AM	Application of surrogate modelling to accelerate design space exploration for catalytic reactor systems; ***Stepan Spatenka***	HYBRID MODELLING FOR THE DYNAMIC SIMULATION OF WATER GAS SHIFT AND METHANOL SYNTHESIS REACTIONS NETWORK; ***Harry Kay***	Towards the complete mineralization of PFOA with a pilot-scale UV-light, boron-nitride—based recirculating reactor unit; ***Juan Donoso***	METHANE PARTIAL OXIDATION (MPO) UNDER PERIODIC REACTION CONDITIONS ON PT/AL_2O_3; ***Surya Solanki***
11:25-11:45 AM	Advantages in the use of AI-based regressions for the kinetic modelling of industrial catalysts; ***Hugo Petremand***	Investigating a Novel Flash Thermal Racemisation Reaction Operated Under Transient Flow Regimes through Kinetic Modelling; ***Harry Kay***		IGNITION THRESHOLD OF ARGON DILUTED METHANE IN ATMOSPHERIC PLASMA-LIQUID MULTIPHASE MICROREACTOR; ***Sudip Das***
11:45-1:15 PM	Lunch on own			
1:15-2:15 PM	Panel Discussion: Vision 2050: Reaction Engineering Roadmap Facilitator: **Ryan Hartman** (NYU) Panelists: **Dan Hickman** (Dow), **Kim McAuley** (Queens University), **Michael Harold** (University of Houston)			
2:15-2:30 PM	Refreshment Break			
	In Honor of the Amundson Awardee: 1 Chairs: Ashish Mhadeshwar (ExxonMobil), Jeffrey Rimer (University of Houston)	**Automation/Digitization in Reaction Engineering: 2** Chairs: Alan Stottlemeyer (Dow), Ram Ratnakar (Shell)	**Reaction Engineering for the Energy Transition: 5** Chairs Jeremy Bedard (Oxy), Nick Thornburg (NREL)	**Novel Reactors and Process Intensification: 5** Chairs: Saurabh Bhandari (Dow), Jiakang Chen (BASF)
2:30-2:50 PM	Reaction Engineering: The ISCRE Board's 2050 Perspective ***Dan Hickman***	Keynote	1071: MICROKINETIC MODELING OF OXIDATIVE COUPLING OF METHANE: CAN ELECTROCHEMISTRY BREAK THE SCALING RELATIONSHIP?; ***Julian Ufert***	Forced Dynamic Operation of Propylene Selective Oxidation to Acrolein in Catalytic Foam Reactor: Reactor Model Development ***Kai Wu***
2:50-3:10 PM	Propane Dehydrogenation in Electrifiable Carbon Membrane Reactor ***Dongxia Liu***	APPLICATION OF DYNAMIC REACTION SCREENING AND DEVELOPMENT OF A 2-	Thermodynamic Analysis Based Programmed Heating Strategies to Limit Carbon Depositions	Can methanol synthesis be enhanced at low pressure with continuous operation?;

		D REACTOR MODEL FOR ACCURATE KINETIC ANALYSIS IN TUBULAR REACTORS; ***Daniel Trahan***	in Electrified Modular Methane Reformer Reactors; ***Collins Don-Pedro***	***Chiara Berretta***
3:10-3:30 PM	Multiple Rate States in Precious Metal Catalyzed Oxidation Reactions: Kinetic Requirements, Multiplicity Features and Rate Determining Steps ***Michael P. Harold***	Model-Based Fault Diagnosis for Closed-loop Feedback controlled Safety-Critical Chemical Reactors: An Experimental Study; ***Pu Du***	ISOPOTENTIAL TITRATION OF AMMONIA ELECTRON TRANSFER ON METAL CATALYSTS; ***Jesse Canavan***	Experimental and modeling of reactive distillation applied for an immobilized enzymatic reaction coated on structured internals; ***Nicolas Chaussard***
3:30-3:50 PM	Refreshment Break			
	In Honor of the Amundson Awardee: 2 Chairs: Ashish Mhadeshwar (ExxonMobil), Jeffrey Rimer (University of Houston)	**Automation/Digitization in Reaction Engineering: 3** Chairs: Alan Stottlemeyer (Dow), Ram Ratnakar (Shell)	**Reaction Engineering for Materials Synthesis** Jeremy Bedard (Oxy), Nick Thornburg (NREL)	**Computational Chemistry and Catalysis, Data Science, ML** Chairs: Saurabh Bhandari (Dow), Jiakang Chen (BASF)
3:50-4:10 PM	Joule heated structured reactors: combining electrification with process intensification ***Enrico Tronconi***	Digital Twin Concept For Hydrogen Production From Biogas; ***Razieh Etezadi***	Mechanistic Insights into Metal-Organic Framework Formation from In-Situ X-Ray Scattering Data ***Gaurav Giri***	COMPUTATIONAL INSIGHTS INTO THE ADSORPTION BEHAVIOR OF H2 AND CO2 ON CU AND ZNO SURFACES FOR METHANOL SYNTHESIS; ***Haseen Siddiqui***
4:10-4:30 PM	Advancing Product Analysis and Polymer Recycling Strategies with Two-Dimensional Gas Chromatography (GC×GC) ***Hilal Ezgi Toraman***	CatTestHub: A Benchmarking Database of Experimental Heterogeneous Catalysis and Insights for Methanol Decomposition; ***Atharva Burte***	A NOVEL PLASMA ENHANCED CHEMICAL VAPOR DEPOSITION (PECVD) REACTOR SYSTEM FOR FABRICATION OF SIC-TYPE CERAMIC FILMS AND MEMBRANES; ***Farnaz Tabarkhoon***	First principles insights into effect of charge condensation on water gas shift reaction mechanism; ***Venkata Rohit Punyapu***
4:30-4:50 PM	Intensification of polyolefin plastic waste hydroconversion in small alkane solvents ***Pavel Kots***	From Laboratory to Pilot: Digital Design Case Study for Cost Effective Catalytic Reactor Scale Up; ***Shahin Goodarznia***	Synthesis of Brightly Fluorescent ZnSe Quantum Dots using Air-Stable Precursors; ***Ali Rad***	Machine Learning for Parametric Sensitivity of Chemical Reactors; ***Joaquin Herrero***

Tuesday, Feb 18: Conference Banquet (18:00-21:30)

Day 3: February 19				
8:15-9:15 AM	Plenary 3: Towards Electrifying Chemical Manufacturing Using Electrolysis *Paul Kenis*			
9:15-9:30 AM	Refreshment Break			
	Room 1	Room 2	Room 3	Room 4
	CO2 Capture and Conversion: 1 Chairs: Gina Noh (Penn State), Sweta Somasi (Dow)	**Biopharmaceutical Reaction Engineering: 1** Chairs: Bryan Patel (Exxon), Jane Shi (Dow)	**General Reaction Engineering: 1** Chairs: Sribala Gorugantu (UH), Sukaran Arora (Dow)	**General Reaction Engineering: 2** Chairs: David Simakov (U. Waterloo), Carsten Sievers (Georgia Tech)
9:30-9:50 AM	Reactive Carbon Capture: Cooperative and Bifunctional Adsorbent-Catalyst Materials and Process Integration for a New Carbon Economy ***Fateme Rezaei***	Development of continuous hydrogenation for pharmaceutical intermediate from Laboratory to Pilot plant;	Academic-Industry Sabbaticals: An Academic Reaction Engineer's Perspective; ***Ryan Hartman***	1093PROXIMITY EFFECTS FOR IMPROVING ETHYL ACETATE SELECTIVITY IN THE DEHYDROGENATIVE COUPLING OF

		Onkar Manjrekar		ETHANOL OVER SUPPORTED CU CATALYSTS; ***Varad Joshi***
9:50-10:10 AM	1019: Barriers to Carbon Dioxide Utilization ***Daniel Hickman***	1055: DEVELOPMENT OF PHARMACEUTICALLY-RELEVANT PHOSPHOLIGANDS FROM LAB TO PLANT VIA MULTI-STAGE FLOW CHEMISTRY; ***Eric Sacia***	1052: Enhancing Accuracy in Particle Resolved CFD Modeling of Fixed Bed Reactors through Integration of Micro-CT and Rigid Body Dynamics; ***Shashank S. Tiwari***	1079: Impact of Intermediate Transfer Rates, Metal Cation Mobility, and Hydrocarbon Pool Mechanisms on the Rates and Selectivity for Tandem CO2 Hydrogenation to Olefins and Fuels; ***Fatima Mahnaz***
10:10-10:30 AM	REACTION PATHWAYS, INTERMEDIATES, AND SITE REQUIREMENTS FOR CO2 METHANATION OVER NI-CE MIXED METAL OXIDES; ***Suchetana Samanta***	DEVELOPMENT AND DEMONSTRATION OF AN ULTRA-HIGH TEMPERATURE CONTINUOUS RACEMIZATION PROCESS FOR RECYCLE OF UNDESIRED ATROPISOMER WASTE STREAM; ***Kiersten Campbell***	CONTROLLING MOLECULAR ARCHITECTURES IN ALKOXYSILANE HYDROLYSIS AND CONDENSATION: REACTOR DESIGN AND PROCESS CONSIDERATIONS; ***Zhichen Shi***	RELATIONSHIP BETWEEN THE OBSERVED REACTION KINETICS OF ETHYLENE TO ETHYLENE OXIDE WITH COMPLEX CHLORINATION AND PROCESS CONDITIONS EFFECT; ***Jake Gold***
10:30-10:45 PM	Refreshment Break			
	CO2 Capture and Conversion: 2 Chairs: Gina Noh (Penn State), Sweta Somasi (Dow)	**Biopharmaceutical Reaction Engineering: 2** Chairs: Bryan Patel (Exxon), Jane Shi (Dow)	**General Reaction Engineering: 3** Chairs: Sribala Gorugantu (UH), Sukaran Arora (Dow)	**General Reaction Engineering: 4** Chairs: David Simakov (U. Waterloo), Carsten Sievers (Georgia Tech)
10:45-11:05 PM	DEVELOPMENT OF DUAL FUNCTION MATERIALS FOR REACTIVE CAPTURE OF CO2 FROM DILUTE STREAM TO PRODUCE CO AT HIGH SELECTIVITY; ***Anh To***	Transport-Kinetic Modeling of a Double N-Debenzylation in the Production of an Active Pharmaceutical Ingredient ***Neda Nazemifard***	PROMOTIONAL ROLE OF ACID SITES ON ALUMINOSILICATE-SUPPORTED; ***Welman Elias***	Optimization of temperature profiles in CO2 methanation reactors by an appropriate selection of catalyst and dilution agent; ***Matteo Percivale***
11:05-11:25 PM	ENHANCED PERFORMANCE OF CU/ZRO2 CATALYSTS IN CO2 HYDROGENATION TO METHANOL; ***Mohd Moiz Khan***	AUTOMATED DISCOVERY OF ENZYMATIC REACTION KINETICS USING SYMBOLIC REGRESSION AND MODEL-BASED DESIGN OF EXPERIMENTS; ***Harry Kay***	CATALYTIC CO-PYROLYSIS OF PYROLYTIC OILY SLUDGE WITH BIOMASS FOR RESOURCE RECOVERY; ***Himanshi Sharma***	Kinetic Modeling and Optimization of a Pharmaceutical Process with Uncertain Inputs; ***Iman Moshiritabrizi***
11:25-11:45 AM	Closing Remarks			