

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 <i>Linda Broadbelt (Northwestern University)</i>			
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 <i>Dion Vlachos (University of Delaware)</i>			
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; <i>M. Doga Tekbas</i>	Keynote: HARNESSING COUPLED REACTION-TRANSPORT PHENOMENA TO DEVELOP STABLE AND SELECTIVE ZEOLITE CATALYSTS FOR OLEFIN OLIGOMERIZATION TO TRANSPORTATION FUELS; <i>Rajamani Gounder</i>	MODELING OF A HEAT-INTEGRATED BIOMASS DOWNDRAFT GASIFIER WITH CONSTRUCTION AND DEMOLITION WASTE AS FEEDSTOCK; <i>Houda Haidar</i>	Microfluidic Laser-Induced Nucleation of Iron (II, III) Oxide Nanoparticle-Doped Supersaturated Aqueous KCl solutions; <i>Kelechi Ndukwe-Ajala</i>
11:05-11:25 AM	Understanding Reaction Environments in Mechanocatalytic Processes; <i>Kinga Golabek</i>	LENGTH EFFECTS ON PRCFD-DERIVED FIXED-BED RADIAL HEAT TRANSFER PARAMETERS; <i>ANTHONY DIXON</i>	Radio Frequency Heating of Catalytic Propane Dehydrogenation: Finite Element Approach, Techno-Economic, and Environmental Assessment. <i>Ankush Rout</i>	Novel modular, layered reactor for continuous, scalable, efficient hydrogenation; <i>Lorenzo Milani</i>
11:25-11:45 AM	H ₂ -Free Conversion of Condensation Polymers with Organic H ₂ Carriers - Kinetic Coupling of Hydrogenolysis and Dehydrogenation Pathways; <i>Manish Shetty</i>	Mechanistic and Kinetic Role of Pd in the Co-Production of Ethylene and Acetic Acid from Ethane over Pd-MoV Oxides; <i>Joseph Lane</i>	CAPITALIZING ON BIPHASIC SYSTEMS FOR THE REACTION WITH IN SITU EXTRACTION OF SUGARS TO FURANS: SOLVENT SELECTION AND REACTION MODELLING; <i>Dominik Soukup-Carne</i>	MECHANISTIC ASPECTS OF SELECTIVE HYDROGEN COMBUSTION (SHC) OVER Na ₂ WO ₄ /SiO ₂ CATALYSTS; <i>Elijah Kipp</i>
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 Chairs: Ryan Hartman (NYU), Moiz Diwan (AbbVie)	Fundamentals of CRE Chairs: 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 NO _x 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 Chairs: Ryan Hartman (NYU), Moiz Diwan (AbbVie)	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 CrO _x /Al ₂ O ₃ 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 <i>Shailendra Bordawekar, AbbVie</i>			
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 <i>Praveen Bollini (University of Houston)</i>			
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 Cattray	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 ₂ O 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 H ₂ AND CO ₂ 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 (Corteva)	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 UNDESIRE 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 (Corteva)	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 ENZYMIC 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			