

2014 AIChE Annual Meeting
Atlanta, GA
Rapid Fire Oral Presentations

Monday, November 17, 2014

Time	Stage 1	Stage 2	Stage 3	Stage 4
6:00pm	566a: Mixed Integer Polynomial Optimisation Vivek Dua, University College London	567b: Quantifying Model Uncertainty in Scarce Data Regions Wei Dai, University of Tulsa	224p: Well to Wheel Life Cycle Assessment of Greenhouse Gas Emissions of Transportation Fuels from Canadian Oil Sands Md Mustafizur Rahman, University of Alberta	231aa: Estimation of the Acentric Factor for Polycyclic Aromatic Hydrocarbons (PAH) and Fullerenes Christopher Pope, Cabrillo College
6:05pm	566f: Higher-Order Inclusions of Nonlinear Systems by Chebyshev Models Benoit Chachuat, Imperial College London	567d: Virtual Kinetics Laboratory for Quantitative Model-Based Discrimination of Reaction Mechanisms Alex Kalos, The Dow Chemical Company	223d: Molecular Descriptor Based Random Forest Predictors of Ionic Liquids Zelimir Kurtanjek, University of Zagreb	231ah: Hydration Free Energies Calculated Using the AMBER ff03 Charge Model for Natural and Unnatural Amino Acids and Multiple Water Models George Khoury, Princeton University
6:10pm	566i: Kinetic Theory for Granular Flow (KTGF) Revisited Yujian Sun, Washington University in St. Louis	568aa: Understanding Cognitive Behavior of Process Operators during Abnormal Situations through Eye Tracker Studies Raj Srinivasan, Institute of Chemical & Engineering Sciences	223x: Towards the Development of a Model for Particle Nucleation Jeffrey Lowe, University of Michigan	231aj: Quantification of Hydrogen Bond Enthalpy and Entropy with COSMO Polarization Charge Densities Andreas Klamt, COSMOlogic GmbH&CoKG
6:15pm	566j: Comprehensive 3D Modeling of Steam Cracking Furnaces: Influence of Flue Gas Radiative Properties, Burner Geometry and Shadow Effects Yu Zhang, Ghent University	568h: Condition Monitoring of a Gasifier in an Integrated Gasification Combined Cycle Plant Pratik Pednekar, West Virginia University	223f: Interfacial Properties of Realistic Molecular Fluids: A Combined Molecular Simulation and Classical Density Functional Theory Approach J. Richard Elliott, The University of Akron	231am: To Dramatically Improve the Ability of CO₂ Capture by Ionic Liquids – Is It a Critical Criterion to Focus in Nano-Scale Wenlong Xie, Nanjing Technical University
6:20pm	566l: Adjoint Model for the Efficient Calculation of Atmospheric Nucleation Sensitivities Sylvia Sullivan, Georgia Institute of Technology	568i: Dynamic Control of Multiple Water Networks for Agile Manufacturing Tianxing Cai, Lamar University	223b: Gibbs Ensemble Simulation of the Phase Diagrams of Simple Fluids: Ar, Kr, and CH₄ Using Temperature Dependent Interaction Parameters Ali Al-matar, KFUPM	231an: Conceptual Process Design for Separation of Rare Gases Using Ionic Liquids Waheed Afzal, University of the Punjab

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6:25pm	<p>566p: Biodetoxification by Lipid Emulsion Droplets: Coarse Grained Molecular Dynamics at the Oil/Water Interface Belinda S. Akpa, University of Illinois at Chicago</p>	<p>568j: Genetic Fuzzy Decoupling of Nonlinear Multiple-Input Multiple-Output Processes Sarah Nikbaksh, Brigham Young University</p>	<p>223ah: Oxygen Reduction Reaction on Pt-Free Catalyst Iron Phthalocyanine Functionalized Graphene for Fuel Cells Sean Mussell, New Mexico Institute of Mining and Technology</p>	<p>231as: Density and Speed of Sound of Binary Mixtures of (Diethyl Malonate + Methanol) at Different Temperatures and Atmospheric Pressure Ricardo Torres, FEI</p>
6:30pm	<p>570ab: Medium-Term Scheduling of an Industrial Multiproduct Batch Plant Esmael Reshid Seid, University of the Witwatersrand</p>	<p>568k: Database Management Method Based on Density and Non-Linearity for Locally Weighted Linear Regression Model Sanghong Kim, Kyoto University</p>	<p>225d: Development and Evaluation of a Novel Non-Traditional Processing Aid for the Pulp and Paper Industry Carter Kirwan, Kemira R&D</p>	<p>231bb: Vapor -Liquid Equilibrium of the Ethyl Acetate and Isoamyl Acetate System at 500 Mbar, 1013.25 Mbar y 1500 Mbar Grace V. de Leon, Universidad Nacional de Colombia</p>
6:35pm	<p>570ac: An Integrated Strategy to Define the Optimal Energy Infrastructure Under Fossil Resources Availability Uncertainty Aldo Vecchiatti, INGAR</p>	<p>568r: Compromise Optimization Tuning Strategy for Model Predictive Controllers Andre S. Yamashita, University of São Paulo</p>	<p>225j: Enhanced Mass Transfer in the Capture of Targets to a Probe Library Consisting of Microbeads with Surface Capture Molecules and Confined in Wells at the Channel Floor of a Microfluidic Cell Setareh Manafirasi, City College of New York</p>	<p>231e: Prediction of Kinematic Viscosities and Vapor-Liquid Equilibria for Ternary Systems Using Activity Coefficient Model Katsumi Tochigi, Nihon University</p>
6:40pm	<p>570b: Application of Better Optimization of Nonlinear Uncertain Systems (BONUS) Algorithm for Adaptive Sensor Placement Rajib Mukherjee, VRI-CUSTOM</p>	<p>568t: A Novel Modeling and Optimization Based Energy Management Solution for Integrated Steel Plants Naresh N. Nandola, ABB Global Industries and Services</p>	<p>153b: Optimal Sizing of Cogeneration (COGEN) System to Manage Flares from Uncertain Sources during Abnormal Process Operations Monzure-Khoda Kazi, Qatar University</p>	<p>231f: The Gibbs-Helmholtz Equation in Chemical Process Technology Paul M. Mathias, Fluor Corporation</p>
6:45pm	<p>570c: Development of the Start-up Procedure for a Thermally Coupled Distillation Columns System through Dynamic Simulation Angela Vasconcelos, Federal University of Campina Grande</p>	<p>568w: An Efficient Control Formulation for Cyclic Process with Application to an Industrial System Naresh N. Nandola, ABB Global Industries and Services</p>	<p>569z: Process Design and Simulation for the Conversion of Coal to Methanol Dwina Candraasih, PT PERTAMINA</p>	<p>231h: A Study on the CO₂ Uptake Behaviour of Supported [Hmim][NTf₂] IL Sorbents Xin Feng, Nanjing Technical University</p>

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6:50pm	<p>570f: Homotopy Continuation Solution Method with Advanced Step Implementation for Nonlinear Model Predictive Control Panos Seferlis, Aristotle University of Thessaloniki</p>	<p>569d: Integrated Solvent and Process Design Exemplified for a Diels-Alder Reaction Teng Zhou, Max Planck Institute for Dynamics of Complex Technical Systems</p>	<p>570s: Saudi Aramco Enterprise-Wide Hydrocarbon Chain Optimization Initiative Ahmed Alshaikh, Saudi Aramco</p>	<p>231i: Phase Behaviour of Ether Alcohol Blends for Reformulated Gasoline Travis P. Benecke, Durban University of Technology</p>
6:55pm	<p>570g: Challenges in the Development of the Mathematical Modeling of a Delayed Coking Process Claudio N. Borges, University of Sao Paulo</p>	<p>569f: Adaptive Energy Management in Renewable Energy Smart Grids Using the Power Grand Composite Curves Approach Athanasios I. Papadopoulos, Centre for Research and Technology-Hellas</p>	<p>570t: Dynamic Simulation Model Based Analysis for Process Development Window of Operability and Control Kadhim Mohammed, Saudi Aramco</p>	<p>231j: Molecular Fundamentals of the Solubility of Gases in Liquid Crystals Bernardo Oyarzún, Delft University of Technology</p>
7:00pm	<p>570h: A Framework for Stochastic Modelling and Optimization of Chemical Engineering Processes Usman Abubakar, University of Aberdeen</p>	<p>569s: Optimization Analysis of a Biorefinery Based on Olive Stone Eulogio Castro, University of Jaén</p>	<p>570z: Distillation Curve Optimization Using Monotonic Interpolation Brenno C. Menezes, Petrobras</p>	<p>231l: A Study on Phase Behavior and Its Application to Cryogenic Technologies for Treatment of Gas Fields with High CO₂ Content Dhanaraj Turunawarasu, Petronas</p>
7:05pm	<p>570j: Analysis of the Anaerobic Digestion Process Using Computational Fluid Dynamics Valentina Hernández, Universidad Nacional de Colombia</p>	<p>569v: Failure Analysis of a Second Generation Biorefinery from Oil Palm Empty Fruit Bunches Using Graph Theory Eulogio Castro, University of Jaén</p>	<p>231v: Application of the Marrero and Pardillo Property Estimation Method to Unsubstituted Polycyclic Aromatic Hydrocarbons (PAH) and Fullerenes Christopher Pope, Cabrillo College</p>	<p>231m: Phase Behaviour and Interfacial Properties of Triangle Well Fluids Angan Sengupta, Indian Institute of Technology, Bombay</p>
7:10pm	<p>570l: Simulation Based Optimization of Stirred Tank Reactors Yuvraj Dewan, CD-adapco</p>	<p>569w: Spatial Modeling of a Tubular Reactor for the High Pressure Synthesis of LDPE Sebastian Fries, TU Darmstadt</p>	<p>231x: Methanol Content in Natural Gas Systems: Modelling with the GC-PR-CPA EoS Martha Hajiw, Heriot Watt University</p>	<p>231o: Sigma Profile Generation with Conceptual Segment Approach M. R. Islam, Lamar University</p>

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7:15pm	570m: Dynamic Analysis of Offshore Natural Gas Processing Plant Lara O. Arinelli, Universidade Federal do Rio de Janeiro	569x: Fast Tracking Process Development Life Cycle Based on State-of-the-Art Process Simulation Models Kadhim Mohammed, Saudi Aramco	231z: Characterization of the Vapour-Liquid Transition of Triangle Well Fluids Confined in Slit Pores Angan Sengupta, Indian Institute of Technology, Bombay	231u: Solubility of CO₂ in Deep Eutectic Solvents: Experiments and Modeling Mohamed K. Hadj-Kali, King Saud University
7:20pm	570af: Efficient Ant Colony Optimization (EACO) Algorithm for Deterministic Optimization Berhane Gebreslassie, Vishwamitra Research Institute			231n: Solubility of Essential Oils in Liquid and Supercritical Carbon Dioxide Odell Glenn Jr. University of South Carolina