Claire S. Adjiman

Monday, October 29, 2018 - 10:06 AM - 10:24 AM, David L. Lawrence Convention Center- 321

58h Systematic Design of Phase-Change Solvents for Post-Combustion CO₂ Capture Based on Advanced Thermodynamics and Holistic Sustainability Assessment Athanasios I. Papadopoulos¹, Gulnara Shavalieva², Felipe Perdomo-Hurtado³, Panos Seferlis¹⁴, Stavros Papadokonstantakis², Claire S. Adjiman³, Amparo Galindo³ and George Jackson³, (1)Chemical Process and Energy Resources Institute, Centre for Research and Technology-Hellas, Thessaloniki, Greece, (2)Department of Space, Earth and Environment, Chalmers University of Technology, Gothenburg, Sweden, (3)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (4)Mechanical Engineering Department, Aristotle University of Thessaloniki, Thessaloniki, Greece

Monday, October 29, 2018, 01:20 PM - 01:45 PM, Westin Convention Center- Washington

139c Improved Efficiency in the Ab Initio Generation of Crystal Structures Isaac Sugden, Imperial College, London, United Kingdom, Claire S. Adjiman, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom and Constantinos C. Pantelides, Process Systems Enterprise Ltd., London, United Kingdom

Tuesday, October 30, 2018 - 02:10 PM - 02:35 PM David L. Lawrence Convention Center- 319

365e Computer-Aided Design of Products Derived from Biomass Pyrolysis Suela Jonuzaj, Nilay Shah and Claire S. Adjiman, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom

Thursday, November 01, 2018 - 10:00 AM - 10:30 AM

626f Investigating the Impact of Water on the Energetics and Kinetics of a Reductive Amination Reaction – a Computational and Experimental Approach Aikaterini Diamanti, Carla Luciani⁷, Jonas Y. Buser⁷, Amparo Galindo⁴ and Claire S. Adjiman⁷, (1)Departamento de Quimica, CUCEI, Universidad de Guadalajara, Guadalajara, Mexico, (2)Eli Lilly and Company, Indianapolis, IN, (3)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom
Benoit Chachuat

Monday, October 29, 2018 - 03:30 PM - 05:00 PM, David L. Lawrence Convention Center- Exhibit Hall B

185af Model-Based Analysis and Optimization of a Semi-Lean MBC Process for Natural Gas Sweetening Ven Chian Quek1,2, Javier Rodriguez3, Nilay Shah1 and Benoit Chachuat1; (1)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (2)Group Research & Technology, Petronas, Kuala Lumpur, Malaysia, (3)Process Systems Enterprise Ltd, London, United Kingdom

Thursday, November 01, 2018 - 02:35 PM - 03:00 PM, David L. Lawrence Convention Center- 316

682f Sustainability Assessment and Targeting in Process Design: A Novel Method Based on Data Envelopment Analysis - Application to Liquid Fuels Daniel F. Rodriguez-Vallejo, Ángel Galán Martín, Benoit Chachuat and Gonzalo Guillén-Gosálbez, Centre for Process Systems Engineering, Imperial College of Science, Technology and Medicine, London, United Kingdom

Friday, November 02, 2018 - 08:51 AM - 09:08 AM, David L. Lawrence Convention Center- 309

734d Model-Based Analysis of a Thermofluidic Engine for Low-Grade Heat Recovery: Accounting for Irreversible Thermal Losses Yukun Wang1, Christos N. Markides2 and Benoit Chachuat1; (1)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (2)Clean Energy Processes Laboratory, Department of Chemical Engineering, Imperial College London, London, United Kingdom

Marc Peter Deisenroth

Tuesday, October 30, 2018 - 05:27 PM - 05:55 PM, David L. Lawrence Convention Center- 303

384d Gaussian Processes for Hybridizing Analytical & Data-Driven Decision-Making Simon Olofsson, Johannes Wiebe, Marc Peter Deisenroth and Ruth Misener, Department of Computing, Imperial College, London, United Kingdom

Amparo Galindo

Thursday, November 01, 2018 - 10:00 AM - 10:30 AM

626f Investigating the Impact of Water on the Energetics and Kinetics of a Reductive Amination Reaction – a Computational and Experimental Approach Aikaterini Diamanti1, Carla
Luciani, Jonas Y. Buser, Amparo Galindo and Claire S. Adjiman, (1)Departamento de Quimica, CUCEI, Universidad de Guadalajara, Guadalajara, Mexico, (2)Eli Lilly and Company, Indianapolis, IN, (3)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom

Monday, October 29, 2018 - 10:06 AM - 10:24 AM, David L. Lawrence Convention Center- 321

58h Systematic Design of Phase-Change Solvents for Post-Combustion CO₂ Capture Based on Advanced Thermodynamics and Holistic Sustainability Assessment Athanasios I. Papadopoulos, Gulnara Shavalieva, Felipe Perdomo-Hurtado, Panos Seferlis, Stavros Papadokonstantakis, Claire S. Adjiman, Amparo Galindo and George Jackson, (1)Chemical Process and Energy Resources Institute, Centre for Research and Technology-Hellas, Thessaloniki, Greece, (2)Department of Space, Earth and Environment, Chalmers University of Technology, Gothenburg, Sweden, (3)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (4)Mechanical Engineering Department, Aristotle University of Thessaloniki, Thessaloniki, Greece

Gonzalo Guillén-Gosálbez

Tuesday, October 30, 2018 - 08:57 AM - 09:16 AM, David L. Lawrence Convention Center- 410

273d Strategic Planning of Supply Chains Considering Extreme Events: Novel Heuristic and Application to the Petrochemical Industry Michael Ehrenstein and Gonzalo Guillén-Gosálbez, Centre for Process Systems Engineering, Imperial College of Science, Technology and Medicine, London, United Kingdom

Thursday, November 01, 2018 - 08:50 AM - 09:15 AM, David L. Lawrence Convention Center- 320

620c Dimensionality Reduction in Sustainability Assessment: A Combined Use of Mixed-Integer Programming and Data Envelopment Analysis Phantisa Limleamthong, Chemical Engineering, Imperial College London, London, United Kingdom and Gonzalo Guillén-Gosálbez, Centre for Process Systems Engineering, Imperial College of Science, Technology and Medicine, London, United Kingdom

Thursday, November 01, 2018 - 02:35 PM - 03:00 PM, David L. Lawrence Convention Center- 316

682f Sustainability Assessment and Targeting in Process Design: A Novel Method Based on Data Envelopment Analysis - Application to Liquid Fuels Daniel F. Rodríguez-Vallejo, Ángel Galán Martín, Benoit Chachuat and Gonzalo Guillén-Gosálbez, Centre for Process Systems Engineering, Imperial College of Science, Technology and Medicine, London, United Kingdom
George Jackson

Monday, October 29, 2018 - 10:06 AM - 10:24 AM, David L. Lawrence Convention Center- 321

**58h Systematic Design of Phase-Change Solvents for Post-Combustion CO₂ Capture Based on Advanced Thermodynamics and Holistic Sustainability Assessment**

_Athanasios I. Papadopoulos^1_, Gulnara Shavalieva^1, Felipe Perdomo-Hurtado^1, Panos Seferlis^1,^4, Stavros Papadokonstantakis^1, Claire S. Adjiman^3, Amparo Galindo^3 and George Jackson^3, (1)Chemical Process and Energy Resources Institute, Centre for Research and Technology-Hellas, Thessaloniki, Greece, (2)Department of Space, Earth and Environment, Chalmers University of Technology, Gothenburg, Sweden, (3)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (4)Mechanical Engineering Department, Aristotle University of Thessaloniki, Thessaloniki, Greece

Monday, October 29, 2018 - 08:18 AM - 08:36 AM, David L. Lawrence Convention Center- 309

**95b Coarse-Grained SAFT-γ Force Fields for the Molecular Modelling of Resins and Asphaltenes**

_Guadalupe Jiménez-Serratos^1_, George Jackson^2, Erich A. Müller^1 and Tim Totton^3, (1)Department of Chemical Engineering, Imperial College London, London, United Kingdom, (2)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (3)BP Exploration Operating Co. Ltd., London, United Kingdom

Monday, October 29, 2018 - 05:00 PM - 05:18 PM, David L. Lawrence Convention Center- 307

**227f The Treatment of Pair Correlations in an Augmented Mean-Field Density Functional Theory of a Simple Model Liquid Crystal**

_Martin Schoen_, Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Berlin, Germany, Andrew J. Haslam, Department of Chemical Engineering, Imperial College London, London, United Kingdom and George Jackson, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom

Niall Mac Dowell

Tuesday, October 30, 2018 - 01:58 PM - 02:20 PM, David L. Lawrence Convention Center- 317

**331e Integrated Power Systems Capacity and Transmission Planning with High Spatial and Temporal Resolution**

_Claras F. Heuberger^1_, Praveen Bains^2 and Niall Mac Dowell^1, (1)Centre for Process Systems Engineering, Centre for Environmental Policy, Imperial College London, London, United Kingdom, (2)Centre for Environmental Policy, Imperial College London, London, United Kingdom
A Mantalaris

Monday, October 29, 2018 - 03:30 PM - 05:00 PM, David L. Lawrence Convention Center- Exhibit Hall B

188an On the Evaluation of the Efficiency of the Chemotherapeutic Agent Gemcitabine on 3D Polymer Based Pancreatic Cancer Models of Various Extracellular Matrix Compositions
Stella Totti1, Mark Allenby2, Susana Brito Dos Santos2, A. Mantalaris2 and Eirini Velljour1, (1)Chemical and Process Engineering, University of Surrey, Guildford, United Kingdom, (2)Chemical Engineering, Imperial College London, London, United Kingdom

Christos N. Markides

Friday, November 02, 2018 - 08:51 AM - 09:08 AM, David L. Lawrence Convention Center- 309

734d Model-Based Analysis of a Thermofluidic Engine for Low-Grade Heat Recovery: Accounting for Irreversible Thermal Losses
Yukun Wang1, Christos N. Markides2 and Benoit Chachuat1, (1)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (2)Clean Energy Processes Laboratory, Department of Chemical Engineering, Imperial College London, London, United Kingdom

Ruth Misener

Tuesday, October 30, 2018 - 08:38 AM - 08:57 AM, David L. Lawrence Convention Center- 409

253c Online Generation Via Offline Selection of Strong Linear Cuts from a Semidefinite Programming Relaxation
Radu Baltean-Lugojan, Imperial College London, London, United Kingdom, Pierre Bonami, IBM, Madrid, Spain, Andrea Tramontani, IBM and Ruth Misener, Department of Computing, Imperial College, London, United Kingdom

Tuesday, October 30, 2018 - 04:22 PM - 04:45 PM, David L. Lawrence Convention Center- 304

363c Stem Cell Biomanufacturing under Uncertainty: A Case Study in Optimizing Red Blood Cell Production
Ruth Misener, Department of Computing, Imperial College, London, United Kingdom

Tuesday, October 30, 2018 - 05:27 PM - 05:55 PM, David L. Lawrence Convention Center- 303

384d Gaussian Processes for Hybridizing Analytical & Data-Driven Decision-Making
Simon Olofsson, Johannes Wiebe, Marc Peter Deisenroth and Ruth Misener, Department of Computing, Imperial College, London, United Kingdom
530b Robust Planning and Scheduling for Processes with Equipment Degradation. Johannes Wiebe and Ruth Misener, Department of Computing, Imperial College, London, United Kingdom.

Erich A. Müller

95b Coarse-Grained SAFT-γ Force Fields for the Molecular Modelling of Resins and Asphaltenes. Guadalupe Jiménez-Serratos, George Jackson, Erich A. Müller, and Tim Totton, (1) Department of Chemical Engineering, Imperial College London, London, United Kingdom, (2) Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (3) BP Exploration Operating Co. Ltd., London, United Kingdom.

Constantinos C. Pantelides

Monday, October 29, 2018 - 01:20 PM - 01:45 PM, Westin Convention Center - Washington


Nilay Shah

Sunday, October 28, 2018 - 04:46 PM - 05:05 PM, David L. Lawrence Convention Center - 409

52e Autologous Cancer Therapies: How Can We Handle the Complexity of the Supply Chain? Maria M. Papathanasiou and Nilay Shah, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom.

Monday, October 29, 2018 - 03:30 PM - 05:00 PM, David L. Lawrence Convention Center - Exhibit Hall B

365e Computer-Aided Design of Products Derived from Biomass Pyrolysis. Suela Jonuzaj, Nilay Shah and Claire S. Adjiman, Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom

507g The Role of Software Tools in Quality By Design: A Case Study on Monoclonal Antibody Production. Maria M. Papathanasiou, Nilay Shah and Efstratios N. Pistikopoulos, (1)Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London, London, United Kingdom, (2)Texas A&M Energy Institute, Texas A&M University, College Station, TX
Luca Mazzei

Monday, October 29, 2018 - 12:30 PM - 12:55 PM, David L. Lawrence Convention Center- 334

165a Experimental and CFD Studies of a New Continuous Process for Mixing of Complex Non-Newtonian Fluids Simona Migliozzi1, Robert Sochon2, Luca Mazzei1 and Panagiota Angeli1, (1)Department of Chemical Engineering, University College London, London, United Kingdom, (2)GlaxoSmithKline, Weybridge, United Kingdom

Monday, October 29, 2018 - 02:35 PM - 03:00 PM, David L. Lawrence Convention Center- 334

165f Experimental and Computational Studies of the Fluid Dynamic Behaviour of Liquid-Solid Mixtures in Agitated Vessels Giovanni Meridiano, Weheliye Hashi Weheliye, Luca Mazzei and Panagiota Angeli, Department of Chemical Engineering, University College London, London, United Kingdom

Monday, October 29, 2018 - 03:30 PM - 05:00 PM, Omni William Penn Hotel- Frick

237s Multifluid Modelling Approaches for the Numerical Investigation of Liquid-Solid Suspensions: Limitations and Challenges Rashid Jamshidi, Giovanni Meridiano, Panagiota Angeli and Luca Mazzei, Department of Chemical Engineering, University College London, London, United Kingdom

Matteo Salvalalglio

Monday, October 29, 2018 - 10:15 AM - 10:30 AM, David L. Lawrence Convention Center- 307

74j On the Interplay between Conformational Complexity, Solution Structure, and Polymorphism in Succinic Acid Nucleation from Solution Ilaria Gimondi and Matteo Salvalalglio, Chemical Engineering, University College London, London, United Kingdom

Friday, November 02, 2018 - 08:30 AM - 08:45 AM, David L. Lawrence Convention Center- 305

739c Combining Biased Sampling and Markov State Models to Characterise the Assembly and Exchange Dynamics of Molecular Materials in Solution Veselina Marinova, Loukas Kollias, Ilaria
Eva Sorensen

Monday, October 29, 2018 - 09:12 AM - 09:30 AM, David L. Lawrence Convention Center- 408

106e Preparing Chemical Engineering Students for the Digitalization of Tomorrow – Integrating Modelling across the Curriculum Eva Sorensen, Department of Chemical Engineering, UCL, London, United Kingdom and Pieter Schmal, Process Systems Enterprise Inc., Cedar Knolls, NJ

Monday, October 29, 2018 - 03:30 PM - 03:48 PM, David L. Lawrence Convention Center- 410

229a Experiences of Embedding Safety throughout a Chemical Engineering Program Eva Sorensen and Michaela Pollock, Department of Chemical Engineering, University College London, London, United Kingdom

Michail Stamatakis

Monday, October 29, 2018 - 04:56 PM - 05:14 PM, David L. Lawrence Convention Center- 402

234e Improving the Efficiency of Kinetic Monte Carlo Simulations for Catalysis with a Parallel Caching Algorithm Michail Stamatakis, Chemical Engineering, University College London, London, United Kingdom

Tuesday, October 30, 2018 - 08:18 AM - 08:36 AM, David L. Lawrence Convention Center- 402

269b Effects of Dopant Loading and CO Adsorption on the Structural Stability of Highly Dilute Alloys Konstantinos Papanikolaou, Matthew Darby and Michail Stamatakis, Chemical Engineering, University College London, London, United Kingdom