Centre for **Process Systems Engineering**

Imperial CPSE Presentations
AIChE Annual Meeting 2018

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 CO_2 Capture Based on Advanced Thermodynamics and Holistic Sustainability Assessment ***Athanasios I. Papadopoulos***[1], *Gulnara Shavalieva*[2], *Felipe Perdomo-Hurtado*[3], *Panos Seferlis*[1,4], *Stavros Papadokonstantakis*[2], *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, 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***[1], *Carla Luciani*[2], *Jonas Y. Buser*[2], *Amparo Galindo*[3] *and Claire S. Adjiman*[3], *(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 Quek[1,2], Javier Rodriguez[3], Nilay Shah[1] and **Benoit Chachuat**[1], (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 Wang**[1], Christos N. Markides[2] and Benoit Chachuat[1], (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 Diamanti**[1], Carla*

Luciani[2], Jonas Y. Buser[2], Amparo Galindo[3] and Claire S. Adjiman[3], (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 CO_2 Capture Based on Advanced Thermodynamics and Holistic Sustainability Assessment ***Athanasios I. Papadopoulos***[1], *Gulnara Shavalieva[2], Felipe Perdomo-Hurtado[3], Panos Seferlis[1,4], Stavros Papadokonstantakis[2], 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*

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. 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*

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 CO_2 Capture Based on Advanced Thermodynamics and Holistic Sustainability Assessment ***Athanasios I. Papadopoulos***[1], *Gulnara Shavalieva*[2], *Felipe Perdomo-Hurtado*[3], *Panos Seferlis*[1,4], *Stavros Papadokonstantakis*[2], *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 ***Clara F. Heuberger***[1], *Praveen Bains*[2] *and Niall Mac Dowell*[2], *(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 Totti[1], Mark Allenby[2], Susana Brito Dos Santos[2], A. Mantalaris[2] and **Eirini Velliou**[1], (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 Wang**[1], Christos N. Markides[2] and Benoit Chachuat[1], (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*

383c 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*

Wednesday, October 31, 2018 - 12:49 PM - 01:08 PM, *David L. Lawrence Convention Center- 409*

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***[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*

Constantinos C. Pantelides

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*

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*

185af Model-Based Analysis and Optimization of a Semi-Lean MBC Process for Natural Gas Sweetening *Ven Chian Quek*[1,2]*, Javier Rodriguez*[3]*, Nilay Shah*[1] *and* ***Benoit Chachuat***[1]*, (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*

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*

Wednesday, October 31, 2018 - 02:36 PM - 02:57 PM, ***Westin Convention Center- Fayette***

507g The Role of Software Tools in Quality By Design: A Case Study on Monoclonal Antibody Production ***Maria M. Papathanasiou***[1]*, Nilay Shah*[1] *and Efstratios N. Pistikopoulos*[2]*, (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*

UCL CPSE Presentations

AIChE Annual Meeting 2018

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 Migliozzi***[1], *Robert Sochon*[2], *Luca Mazzei*[1] *and Panagiota Angeli*[1], *(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*

*Gimondi and **Matteo Salvalalglio**, Chemical Engineering, University College London, London, United Kingdom*

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*