



**ESCAPE-27** Barcelona  
October 1<sup>st</sup> - 5<sup>th</sup> 2017  
European Symposium on Computer-Aided  
Process Engineering



## **European Symposium on Computer-Aided Process Engineering**

**Fira de Barcelona, Hall 8, Barcelona, Spain**

**01 – 05 October, 2017**

**Scientific Program**

(updated: September 18<sup>th</sup>, 2017)

[\(Link 1: map\)](#)

[\(Link 2: view\)](#)





## 01, Sunday

**09:00 - 14:00 || CAPE-WP Business Meeting** (by invitation)

Room: E2 (2<sup>nd</sup> floor)

**15:30 - 18:00 || Registration**

Desk

**17:00 - 19:00 || Welcome Address and Cocktail**

Main Hall of the Congress Venue



## 02, Monday

### 08:00 - 16:30 || Registration

Desk

### 08:00 - 18:00 || Posters

#### Poster Hall (P1)

#### T1.- Modeling and Simulation

- P1.01 CFD Simulation of Spray Drying with Ultrasonic Dispersion 25  
**Evgeniy Lebedev, Mariya Gordienko, Alexander Troyankin and Natalia Menshutina (Evgeniy Lebedev)**
- P1.02 Size-Based Particle Separation in Coiled Channel Flow of Non-Circular Cross-Section 31  
**Jakob D. Redlinger-Pohn and Stefan Radl (Jakob D. Redlinger-Pohn)**
- P1.03 Methodology and Pitfalls when Calibrating a PBM: the Case of Twin-Screw Wet Granulation 43  
**Daan Van Hauwermeiren, Maxim Verstraeten, Thomas De Beer and Ingmar Nopens (Daan Van Hauwermeiren)**
- P1.04 A CAPE-Taguchi combined method to optimize a NPK fertilizer plant including population balance modeling of granulation-drying rotary drum reactor 49  
**Carlos Herce, Antonia Gil, Miguel Gil and Cristóbal Cortés (Carlos Herce)**
- P1.05 Local vs Global Estimability Analysis of Population Balance Models for Crystallization Processes 55  
**Dimitrios Fysikopoulos, Akos Borsos, Wei Li, Iyke I. Onyemelukwe, Brahim Benyahia, Zoltan K. Nagy and Chris D. Rielly (Dimitrios Fysikopoulos)**
- P1.06 Rate-based hydrodynamics and reaction performance of a high-pressure reactive distillation column for the production of biodiesel fuel 103  
**Mayra Margarita May-Vázquez, Fernando I. Gómez-Castro, Mario Alberto Rodríguez-Ángeles and Ramiro Rivera-Aguilera (Fernando Gomez-Castro)**
- P1.07 Sequential-based process modelling of a circulating fluidized bed reactor 109  
**Hasan Jafari, Amir Sheikhi and Rahmat Sotudeh-Gharebagh (Rahmat Sotudeh-Gharebaagh)**
- P1.08 Modelling of an adiabatic trickle-bed reactor with phase change 115  
**Carlos Eduardo Ramírez-Castelán, Angélica Hidalgo-Vivas, Jacob Brix, Anker D. Jensen and Jakob K. Huusom (Carlos Eduardo Ramirez Castelan)**
- P1.09 Model of an Industrial Reactor for Formaldehyde Production with Catalyst Deactivation 121  
**Catarina G. Braz, Henrique A. Matos, A. Mendes, Jorge F. Rocha and Ricardo P. Alvim (A. Catarina Braz)**
- P1.12 Model Based Estimation of 2D Crystallization Kinetics from Concentration and CLD Measurements 169  
**Botond Szilagyi, Akos Borsos, Elena Simone and Zoltan K. Nagy (Botond Szilagyi)**
- P1.13 Molecular Dynamics Simulations of Gas-Expanded Liquids 175  
**Emanuel Granero Fernandez, Jean-Stéphane Condoret, Vincent Gerbaud and Yaocihuatl Medina-Gonzalez (Emanuel Granero Fernandez)**
- P1.14 Prediction of structure changes of organic-silica aerogels during pyrolysis 181  
**Mariia Gordienko, Dmitriy Belous, Andrey Tyrtshnikov, Igor Mitrofanov, Natalia Menshutina and Evgeniy Lebedev (Mariia Gordienko)**



P1.15	Dynamic hybrid model for ultrafiltration membrane processes <b>Victor Hugo Grisales Diaz, Oscar Andrés Prado-Rubio, Mark J. Willis and Moritz von Stosch (<u>Victor Hugo Grisales Diaz</u>)</b>	193
P1.16	Software Tool for Computing and Visualization of Enhanced Residue Curve Maps <b>Valentin Plesu, Hector Cruzado Valverde, David Curco, Alexandra Elena Bonet-Ruiz, Jordi Bonet, Petrica Iancu and Joan Llorens (<u>Valentin Plesu</u>)</b>	199
P1.17	A Systematic Identification Method for Thermodynamic Property Modelling <b>Olivia A. Perederic, Larissa P. Cunico, Bent Sarup, John M. Woodley and Rafiqul Gani (<u>Olivia A. Perederic</u>)</b>	205
P1.18	Numerical models for phase transition of polymers used in latent heat thermal energy storages <b>Klemens Marx, Andreas Sommer, Wolfgang Hohenauer and Tilman Barz (<u>Klemens Marx</u>)</b>	211
P1.19	Characterisation of axial dispersion in a Meso-scale Oscillatory Baffled Crystalliser using a Numerical Approach <b>Emmanuel N. Kimuli, lyke I. Onyemelukwe, Brahim Benyahia and Chris D. Rielly (<u>Emmanuel Kimuli</u>)</b>	223
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P1.21	Evaluation of the accuracy of modelling the separation of highly non-ideal mixtures: extractive heterogeneous-azeotropic distillation <b>Andras Jozsef Toth, Eniko Haaz, Tibor Nagy, Renata Tari, Ariella Janka Tarjani, Daniel Fozer, Agnes Szanyi, Katalin-Angyal Koczka, Laszlo Racz, Gergely Ugro and Peter Mizsey (<u>Andras Jozsef Toth</u>)</b>	241
P1.22	Managing supply chain disruptions: an integrated agent-oriented approach <b>Behzad Behdani and Rajagopalan Srinivasan (<u>Behzad Behdani</u>)</b>	595

## Poster Hall (P2)

### T2.- Synthesis and Design

P2.01	Stochastic Multi-Objective Process Optimization by using the Composite Objective Function <b>Žan Zore, Klavdija Zirngast, Zorka Novak Pintarič and Zdravko Kravanja (<u>Žan Zore</u>)</b>	601
P2.02	A Mixed Integer Linear Programming (MILP) Model for Optimal Operation of Industrial Resource Conservation Networks (RCNs) under Abnormal Conditions <b>Raymond R. Tan, Dominic C. Y. Foo, Santanu Bandyopadhyay, Kathleen B. Aviso and Denny Kok Sum Ng (<u>Raymond Tan</u>)</b>	607
P2.03	Integrated Synthesis of Batch Plants and Utility Systems <b>Ludger Holters, Björn Bahl, Matthias Lampe, Maike Hennen and André Bardow (<u>Ludger Holters</u>)</b>	625
P2.04	Infeasible Path Global Flowsheet Optimization Using McCormick Relaxations <b>Dominik Bongartz and Alexander Mitsos (<u>Dominik Bongartz</u>)</b>	631
P2.05	A MOO approach towards sustainable process design: integrating the three pillars of sustainability <b>Federico Scotti, Nicola Fabricatore, Piernico Sepiacci and Davide Manca (<u>Federico Scotti</u>)</b>	637
P2.06	Modelling of the hydrotreating process to produce renewable aviation fuel from micro-algae oil <b>Alejandra Gómez-De la Cruz, Araceli G. Romero-Izquierdo, Claudia Gutiérrez-Antonio, Fernando I. Gómez-Castro and Salvador Hernández (<u>Claudia Gutiérrez-Antonio</u>)</b>	655
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- P2.08 *Optimal synthesis of integrated process for co-production of biodiesel and hydrotreated vegetable oil (HVO) diesel from hybrid oil feedstocks* 673  
**Carlo Edgar Torres-Ortega, Jian Gong, Fengqi You and Ben-Guang Rong (Carlo Edgar Torres-Ortega)**
- P2.09 *Synthesis of a Biomass-to-Liquids (BTL) Process using a Hybrid Pyrolysis-Gasification System* 691  
**Bilal Patel and Xinying Liu (Bilal Patel)**
- P2.10 *A Framework for an Optimized Sustainable Product and Process Design: Acetone-Butanol-Ethanol Separation and Purification* 697  
**Nematihuani Morales-Espinosa, Eduardo Sánchez-Ramírez, Juan José Quiroz-Ramírez, Juan Gabriel Segovia-Hernández, Fernando I. Gómez-Castro and Ricardo Morales-Rodríguez (Ricardo Morales-Rodríguez)**
- P2.11 *Feasibility Study of New Synthesis Route of Tetraethoxysilane from Rice Hull Ash* 703  
**Thuy T. H. Nguyen, Sho Kataoka, Norihisa Fukaya, Kazuhiko Sato, Jun-Chul Choi and Akira Endo (Thuy Nguyen)**
- P2.12 *Two-stage Stochastic Optimization of Carbon Dioxide Supply Chain and Utilization Model through Carbon Dioxide Capturing Process* 727  
**Narut Suchartsunthorn and Kitipat Siemanond (Narut Suchartsunthorn)**
- P2.13 *Topside process design for the liquid CO<sub>2</sub> Injection* 733  
**Umer Zahid, Yong Heon Kim and Usama Ahmed (Umer Zahid)**
- P2.14 *Optimal Structure Synthesis of Ternary Distillation Processes Using a Stepwise VLE Description* 739  
**Hiroshi Takase, Richard D. Braatz and Shinji Hasebe (Hiroshi Takase)**
- P2.15 *Planning of biobutanol production considering raw material availability: economic and environmental optimization* 757  
**Juan José Quiroz-Ramírez, Eduardo Sánchez-Ramírez and Juan Gabriel Segovia-Hernández (Juan Gabriel Segovia-Hernandez)**
- P2.16 *Targeting and Design of Organic Rankine Cycle Systems for Multiple Heat Sources with Simultaneous Working Fluid Selection* 769  
**Mirko Z. Stijepovic, Athanasios I. Papadopoulos, Patrick Linke, Vladimir Stijepovic, Aleksandar S. Grujic, Mirjana Kijevčanin and Panos Seferlis (Mirko Z. Stijepovic)**
- P2.17 *Heat Exchanger Network Retrofit with Fouling Effects* 775  
**Supapol Rangfak and Kitipat Siemanond (Supapol Rangfak)**
- P2.18 *Multi-objective optimization of utility systems and heat exchanger networks: method and application to the solar-assisted hydrothermal gasification case* 781  
**Alberto Mian, Adriano V. Ensinas, Emanuele Martelli and François Maréchal (Alberto Mian)**
- P2.19 *Modelling, Simulation and Economical Evaluation of Dry Food Manufacture at Different Production Scales.* 787  
**Alberto Almena, Estefanía Lopez-Quiroga, Constantinos Theodoropoulos, Peter J. Fryer and Serafim Bakalis (Alberto Almena)**
- P2.20 *Heat Exchanger Design Optimization Considering Threshold Fouling Modelling* 799  
**André L. H. Costa, Julia C. Lemos and Miguel J. Bagajewicz (André Costa)**
- P2.21 *Design of a New Sustainable Methanol Plant Coupled to an Ethanol Distillery* 805  
**Lucas B. Rocha, Marcelino L. Gimenes, Sergio H. B. Faria, Laureano Jiménez and Thiago Cavali (Lucas Rocha)**
- P2.22 *Synthesis of a New Route for Methanol Production by Syngas Arising from Sugarcane Vinasse* 811  
**Rodrigo O. Silva, Henryck C. M. H. Yoshi, Lucas B. Rocha, Oswaldo C. M. Lima, Laureano Jiménez and Luiz M. M. Jorge (Laureano Jiménez)**



## Poster Hall (P3)

### T3.- Planning and Scheduling

- P3.01 *Enterprise-Wide Optimization for Operations of Crude-Oil Refineries: Closing the Procurement and Scheduling Gap* 1249  
**Brenno C. Menezes, Ignacio E. Grossmann and Jeffrey D. Kelly (Brenno Menezes)**
- P3.02 *Condition-based operational optimization of industrial combined heat and power plants under time-sensitive electricity prices* 1261  
**Egidio Leo and Sebastian Engell (Egidio Leo)**
- P3.03 *A Novel Decision-Making Approach for Supplier Selection under Risks* 1267  
**Samira Mokhtar, Parisa A. Bahri, Sorousha Moayer and Adrian James (Samira Mokhtar)**
- P3.04 *Optimal Planning of a Solar Cells Manufacturing System involving Economic Aspects* 1279  
**Sergio Castellanos, José Ezequiel Santibañez-Aguilar and Antonio Flores-Tlacuahuac (José Ezequiel Santibañez-Aguilar)**
- P3.05 *Inventory planning and control in 'green' pharmacies supply chains – A System Dynamics modelling perspective* 1285  
**Naoum Tsolakis and Jagjit Singh Srari (Naoum Tsolakis)**
- P3.06 *Multiperiod and Multiproduct Model for the Optimal Production Planning in the Gases Sector: Application to an Industrial Case Study* 1297  
**David Fernández, Carlos Pozo, Ruben Folgado and Laureano Jiménez (David Fernández)**
- P3.07 *Optimal Production Planning and Crude Oil Blending in a Conventional Oilfield* 1309  
**Ana C. Duckwen, M. Susana Moreno, Daniel O. Borio and J. Alberto Bandoni (Ana C. Duckwen)**
- P3.08 *Optimal planning of energy production involving carbon capture systems through a multi-stakeholder scheme.* 1315  
**Aurora de Fatima Sanchez-Bautista, José Ezequiel Santibañez-Aguilar, J. Betzabe González-Campos and José María Ponce-Ortega (Aurora de Fatima Sanchez-Bautista)**
- P3.09 *A Bi-objective two step Simulated Annealing Algorithm for Production Scheduling* 1351  
**Nelson Chibeles-Martins, António Marques and Tânia Pinto-Varela (Nelson Chibeles-Martins)**
- P3.10 *Tank Management in a Multi-Product Bottling Facility* 1357  
**Alexandros Koulouris and Konstantinos Kokonas (Alexandros Koulouris)**
- P3.11 *Energy-Efficient and Labor-Aware Production Scheduling based on Multi-Objective Optimization* 1369  
**Xu Gong, Toon De Pessemer, Luc Martens and Wout Joseph (Xu Gong)**
- P3.12 *Resource-Constrained Formulation for Production Scheduling and Maintenance* 1375  
**Adrian M. Aguirre and Lazaros G. Papageorgiou (Adrian Aguirre)**
- P3.13 *A decomposition algorithm for the simultaneous batching and scheduling of multistage batch facilities* 1393  
**Yanina Fumero, Gabriela Corsano and Jorge M. Montagna (Yanina Fumero)**
- P3.14 *Towards a software engineering approach to the deployment and implementation of scheduling systems* 1405  
**Gabriela P. Henning (Gabriela P. Henning)**
- P3.15 *An Efficient Way to Tackle Uncertainty in the Scheduling of a Continuous Evaporation System* 1411  
**Carlos G. Palacín, José Luis Pitarch, César de Prada and Carlos Alberto Méndez (José Luis Pitarch)**
- P3.16 *Recovery Scheduling for Industrial Processes Using Graph Constraints* 1417  
**Muhammed Bahadir Saltik, Sander van Gameren, Leyla Özkan and Siep Weiland (Sander van Gameren)**
- P3.17 *The Application of Reservoir Simulation to the Optimization of Shale Gas Supply Chain Design and its Water Management Structure* 1435  
**Jorge Chebeir, Hope Asala, Arash Dahi Taleghani and Jose A. Romagnoli (Jorge Chebeir)**



- P3.18 *Optimal Design of Multi-Enterprise Industrial Waste-to-Energy Networks* 1441  
**Vasco Bolis, Elisabet Capón-García and Konrad Hungerbühler (Vasco Bolis)**
- P3.19 *CLSC design with simultaneous consideration of product design for manufacturing and remanufacturing* 1453  
**Luis Javier Zeballos, Carlos Alberto Méndez and Ana Paula Barbosa-Póvoa (Luis Javier Zeballos)**

## Poster Hall (P6)

### T6.- Concepts, Methods and Tools

- P6.01 *Process Optimization by Applying a Simultaneous Dynamic Method* 2047  
**Alexander Zinser, Liisa Rihko-Struckmann and Kai Sundmacher (Alexander Zinser)**
- P6.02 *On the Solution of the PBE by Orthogonal Expansion of the Maximum Entropy Functional* 2053  
**Menwer Attarakih, Abdelmalek Hasseine and Hans-Jörg Bart (Menwer Attarakih)**
- P6.03 *Enhanced Surrogate Assisted Global Optimization Algorithm Based on Maximizing Probability of Improvement* 2065  
**Roymel R. Carpio, Roberto C. Giordano and Argimiro R. Secchi (Argimiro Secchi)**
- P6.04 *The Adjoint Method for Gradient-based Dynamic Optimization of UV Flash Processes* 2071  
**Tobias K. S. Ritschel, Andrea Capolei and John Bagterp Jørgensen (John Bagterp Jørgensen)**
- P6.05 *Integration of Design, Control and Scheduling: A Dynamic Optimization Framework for Multi-product Chemical Processes under Disturbances and Uncertainty* 2077  
**Robert Koller and Luis Ricardez-Sandoval (Luis Ricardez-Sandoval)**
- P6.06 *Assessment of the Accuracy and Dynamic Simulation Capabilities of Liquid-Vapour Two-Phase Flow Separated and Mixture Models* 2095  
**Rodrigo G. D. Teixeira and Argimiro R. Secchi (Argimiro Secchi)**
- P6.07 *Optimisation of Batch Extractive Distillation Process with Entrainer Recycle* 2101  
**Laszlo Hegely and Peter Lang (Laszlo Hegely)**
- P6.08 *Efficient global optimization of a novel hydroformylation process* 2113  
**Tobias Keßler, Nick Mertens, Christian Kunde, Corina Nentwich, Dennis Michaels, Sebastian Engell and Achim Kienle (Tobias Keßler)**
- P6.09 *Deterministic and Stochastic Optimization of Acid Pretreatment for Lignocellulosic Ethanol Production* 2149  
**Sumit Kumar Verma and Yogendra Shastri (Sumit Verma)**
- P6.10 *A New Disjunctive Formulation for the Simultaneous Optimization and Heat Integration with Cold/Hot and Unclassified Streams* 2167  
**Natalia Quirante, José A. Caballero and Ignacio E. Grossmann (Natalia Quirante)**
- P6.11 *Developing a Multi-Objective Strategic-Tactical Optimization Model for Sustainable Production Supply Chains Considering Electricity Cogeneration: Sugar Cane Bioenergy Industry* 2179  
**Shabnam Morakabatchiankar, Kefah Hjaila, Moisés Graells and Antonio Espuña (Shabnam Morakabatchiankar)**
- P6.12 *Application of Genetic Algorithm to Layer Patterning of Plate Fin Heat Exchanger* 2185  
**Seung-Kwon Seo, Du-Hyeon Cho, Youngsub Lim and Chul-Jin Lee (Seung-Kwon Seo)**
- P6.13 *Multi-objective Optimization of a Batch Transesterification Reactor Considering Reactor and Methanol Separation Unit Together* 2203  
**Riju De, Sharad Bhartiya and Yogendra Shastri (Riju De)**
- P6.14 *Selection of a minimum toxicity and high performance ionic liquid mixture for the separation of aromatic - aliphatic mixtures by extractive distillation* 2209  
**Ismael Díaz, Manuel Rodriguez and Emilio J. González (Díaz Ismael)**





## Poster Hall (P7)

### T7.- CAPE applications addressing Global Grand Challenges

- P7.01 *Optimal design of urban energy systems with demand side management and distributed generation* 2371  
**Stéphane Crémel, Miao Guo, Gonzalo Bustos-Turu, Koen H. van Dam and Nilay Shah (Stéphane Crémel)**
- P7.02 *Trade-offs in the Design of Urban Energy Systems* 2383  
**Kamal Kuriyan and Nilay Shah (Kamal Kuriyan)**
- P7.03 *A three-stage stochastic optimization model for the design of smart energy districts under uncertainty* 2389  
**Matteo Zatti, Emanuele Martelli and Edoardo Amaldi (Matteo Zatti)**
- P7.04 *Design and operational scheduling of power systems incorporating interconnection options* 2395  
**Nikolaos E. Koltsaklis and Michael C. Georgiadis (Nikolaos Koltsaklis)**
- P7.05 *Rigorous synthesis of energy supply systems by time-series aggregation* 2413  
**Björn Bahl, Julian Lützwow, Dinah Elena Majewski, Matthias Lampe, Maïke Hennen and André Bardow (Björn Bahl)**
- P7.06 *Comparison of Energy Performance of Organic Rankine and Kalina Cycles Considering Combined Heat Sources at Different Temperature* 2419  
**Mengying Wang, Xiao Feng and Yufei Wang (Wang Mengying)**
- P7.07 *Managing Uncertain Industrial Flares during Abnormal Process Operations using an Integrated Optimization and Monte Carlo Simulation Approach* 2425  
**Monzure-Khoda Kazi, Fadwa Eljack and Vasiliki Kazantzi (Vasiliki Kazantzi)**
- P7.08 *A Mathematical Technique for Optimal Design of Hybrid Power Systems Considering Demand-side Management* 2431  
**Jui-Yuan Lee, Li-Hua Tseng and Cheng-Liang Chen (Jui-Yuan Lee)**
- P7.09 *A MILP model for the design of multi-energy systems with long-term energy storage* 2437  
**Paolo Gabrielli, Matteo Gazzani, Emanuele Martelli and Marco Mazzotti (Paolo Gabrielli)**
- P7.10 *The Impact of Novel and Conventional Working Fluids on the Control Performance in Organic Rankine Cycles* 2443  
**Theodoros Zarogiannis, Athanasios I. Papadopoulos, Panos Seferlis and Patrick Linke (Theodoros Zarogiannis)**
- P7.11 *Operation Data based Modelling and Optimization of Thermal Power Units under Full Working Conditions* 2455  
**Tianxiao Li, Pei Liu and Zheng Li (Tianxiao Li)**
- P7.12 *Lessons Learnt from Alarm Management in a Combined-Cycle Gas Turbine Power Plant* 2461  
**Jay Sompura, Parag Shankar, Gamit S, Babji Srinivasan and Rajagopalan Srinivasan (Babji Srinivasan)**
- P7.13 *Energy Management Strategies for RES-enabled Smart-grids empowered by an Internet of Things (IoT) Architecture* 2473  
**Chrysovalantou Ziogou, Spyros Voutetakis and Simira Papadopoulou (Chrysovalantou Ziogou)**
- P7.14 *Modelling and Optimal Operation of a Crude Oil Hydrotreating Process with Atmospheric Distillation Unit Utilising Stacked Neural Networks* 2479  
**Wissam Muhsin and Jie Zhang (Wissam Muhsin)**
- P7.15 *Assessing Technological Options in Biomass-Based Energy Supply Chains through a Quantitative Methodology for Risk and Regret Evaluation* 2491  
**Federico d'Amore and Fabrizio Bezzo (Federico d'Amore)**



- P7.16 *Potential of Milking of Microalgae Grown on Biofilm Photobioreactor for Renewable Hydrocarbon Production* 2497  
**Sofia Chaudry, Parisa A. Bahri and Navid R. Moheimani (Parisa Arabzadeh-Bahri)**
- P7.17 *Process Modeling of Fluidized Bed Biomass-CO<sub>2</sub> Gasification using ASPEN Plus* 2509  
**Narendra Sadhwani, Pengcheng Li, Mario R. Eden and Sushil Adhikari (Narendra Sadhwani)**
- P7.18 *Process Simulation and Economic Analysis of Producing Liquid Transportation Fuels from Biomass* 2515  
**Pengcheng Li, Narendra Sadhwani, Zhihong Yuan and Mario R. Eden (Pengcheng Li)**
- P7.19 *Dynamic Modelling and Experimental Validation of Mass Flow in a Pilot-Scale Pretreatment Continuous Tubular Reactor* 2521  
**Felicia Rodríguez, Ismael Jaramilo, Ricardo Jara and Arturo Sanchez (Arturo Sanchez)**
- P7.20 *Optimal Design and Operation of Heat Networks Utilising Hydrogen as an Energy Carrier* 2527  
**André Prates Pereira and Sheila Samsatli (Andre Prates Pereira)**
- P7.21 *Solar Hydrogen Production via Aqueous Methanol Electrolysis* 2533  
**Harvey Arellano-Garcia, Maximilian Robert Ife and Mohammed Sanduk (Maximilian Robert Ife)**
- P7.22 *Cluster Analysis of Process Operational Data to Identify Representative Scenarios for Pinch Analysis and Energy Optimisation Studies* 2539  
**V. E. Araújo, Fernando P. Bernardo, C.M. Reis and F.G. Martins (V. E. Araújo)**
- P7.23 *Multi-objective optimization of the water scrubbing process for biogas upgrading* 2551  
**Francesco Magli, Federico Capra, Giulio Bortoluzzi, Emanuele Martelli and Manuele Gatti (Manuele Gatti)**
- P7.24 *Application of Cryogenic Energy Storage to Liquefied Natural Gas Regasification Power Plant* 2557  
**Jinwoo Park, Inkyu Lee, Hyungjoon Yoon, Jiyong Kim and Il Moon (Jinwoo Park)**
- P7.25 *Dynamic modelling of a hybrid diabatic compressed air energy storage and wind turbine system* 2569  
**He Jin, Pei Liu and Zheng Li (He Jin)**
- P7.26 *Modelling of the Thermal Performance of SGSP using COMSOL Multiphysics* 2575  
**Argyrios Anagnostopoulos, Alasdair Campbell and Harvey Arellano-Garcia (Argyrios Anagnostopoulos)**
- P7.27 *Capacity Fade Minimizing Model Predictive Control Approach for the Identification and Realization of Charge-Discharge Cycles in Lithium Ion Batteries* 2581  
**Resmi Suresh and Raghunathan Rengaswamy (Resmi Suresh)**



## 09:00 - 10:00 || Opening / Awards

### Main Auditorium

## 10:00 - 11:00 || ESCAPE / WCCE Plenary

### Main Auditorium

- 10:00 *Evolution of Process Systems Engineering and Future Trends in Research* 1  
**Ignacio E. Grossmann**  
*Rudolph R. and Florence Dean University Professor*  
*Center for Advanced Process Decision Making - Department of Chemical Engineering*  
*Carnegie Mellon University, Pittsburgh, USA*

## 11:00 - 11:45 || Posters / Coffee Break

### Hall

## 11:50 - 12:50 || ESCAPE Keynotes

### Room B4

Chairpersons: Prof. Ana Barbosa-Povoa and Prof. Fengqi You

### T3.- Planning and Scheduling

- 11:50 *Continuous-Time Heuristic Model for Medium-Term Capacity Planning of a Multi-Suite, Multi-Product Biopharmaceutical Facility* 1303  
**Karolis Jankauskas, Lazaros G. Papageorgiou and Suzanne S. Farid (Karolis Jankauskas)**
- 12:20 *Rolling Horizon Condition-based Planning of Production and Utility Systems in Process Industries* 1333  
**Nur I. Zulkafli and Georgios M. Kopanos (Georgios M. Kopanos)**

### Room C5

Chairpersons: Prof. Cesar De Prada and Dr. Iiro Harjunkoski

### T4.- Process monitoring and control

- 11:50 *IQC analysis of constrained MPC of large-scale systems* 1627  
**Panagiotis Petsagkourakis, William Heath and Constantinos Theodoropoulos (Constantinos Theodoropoulos)**
- 12:20 *Coordination of distributed MPC systems through dynamic real-time optimization with closed-loop prediction* 1603  
**Hao Li and Christopher L.E. Swartz (Christopher L.E. Swartz)**

### Room C1

Chairpersons: Prof. Valentin Plesu and Prof. Edwin Zondervan

### T2.- Synthesis and Design

- 11:50 *New Method and Software for Computer-Aided Flowsheet Design and Analysis* 649  
**Anjan K. Tula, Rafiqul Gani and Mario R. Eden (Anjan Tula)**

### T7.- CAPE applications addressing Global Grand Challenges

- 12:20 *Challenges and Potentials of Modelling Tools Total Site Integration and Utility System Optimisation* 2545  
**Petar Sabev Varbanov, Jiří Jaromír Klemeš and Ferenc Friedler (Petar Sabev Varbanov)**



## 13:00 - 14:30 || Lunch

Catering Area

## 13:00 - 14:30 || EURECHA – Annual General Meeting (by invitation)

Room: E6 (2<sup>nd</sup> floor)

## 14:30 - 15:30 || ESCAPE / WCCE Plenary

Room C1

Chairperson: Prof. Rafiqul Gani

- 14:30 *Prospects and Challenges for Process Systems Engineering in Healthcare* 3  
**Gintaras V. (Rex) Reklaitis**  
*Burton and Kathryn Gedge Distinguished Professor of Chemical Engineering*  
*Davidson School of Chemical Engineering*  
*Purdue University, West Lafayette, USA*

## 15:30 - 16:25 || Posters / Coffee Break

Hall

## 16:30 - 18:50 || ESCAPE Lectures

Room C5

Chairpersons: Prof. Flavio Manenti and Prof. Yu Qian

### T1.- Modeling and Simulation

- 16:30 *Systematic Generation of Chemical Reactions and Reaction Networks subject to Energetic Constraints* 133  
**Carolina S. Vertis, José F. O. Granjo, Nuno M. C. Oliveira and Fernando P. Bernardo (Carolina Vertis)**
- 16:50 *A two-layer identification strategy for the development of stochastic models of the travelling traders' exchange problem* 265  
**Chunbing Huang, Patrick M. Piccione, Federica Cattani and Federico Galvanin (Chunbing Huang)**
- 17:10 *Identifiability of the glyceride transesterification kinetics via alkaline catalysis* 289  
**José F. O. Granjo, Belmiro P. M. Duarte and Nuno M. C. Oliveira (Jose Granjo)**
- 17:30 *Constrained Global Sensitivity Analysis: Sobol' indices for problems in non-rectangular domains* 151  
**Oleksiy V. Klymenko, Sergei Kucherenko and Nilay Shah (Oleksiy V. Klymenko)**
- 17:50 *Design of Optimal Experiments for Dynamic MIMO Identification* 319  
**Kurt-Erik Häggblom (Kurt-Erik Häggblom)**
- 18:10 *Model-based design of experiments under structural model uncertainty* 145  
**Marco Quaglio, Eric S. Fraga and Federico Galvanin (Marco Quaglio)**
- 18:30 *A Novel Approach for Risk Minimization in Life-Cycle Oil Production Optimization* 157  
**Andrea Capolei, Lasse Hjuler Christiansen and John Bagterp Jørgensen (Lasse Hjuler Christiansen)**



**Room B4**

**Chairpersons: Prof. Mariano Martin and Prof. Karl Tapio Westerlund**

**T2.- Synthesis and Design**

- 16:30 *Design and Operation of a Supply Chain Model for Electric and Plug-in Hybrid Electric Vehicles: Snapshot Model* 883  
**Alberto Betancourt-Torcat, Tuhin Poddar and Ali Almansoori (Ali Almansoori)**
- 16:50 *Techno-economic assessment of the effects of biogas rate fluctuations on industrial applications of solid-oxide fuel cells* 895  
**Sonja Sechi, Sara Giarola, Andrea Lanzini, Marta Gandiglio, Gbemi Oluleye, Massimo Santarelli and Adam Hawkes (Sara Giarola)**
- 17:10 *Designing Integrated Biorefineries Supply Chain: Combining Stochastic Programming Models with Scenario Reduction Methods* 901  
**Helena Paulo, Teresa Cardoso-Grilo, Susana Relvas and Ana Paula Barbosa-Póvoa (Helena Paulo)**
- 17:30 *Location-dependent optimal biorefinery synthesis* 907  
**Maria-Ona Bertran, John M. Woodley and Rafiqul Gani (Maria-Ona Bertran)**
- 17:50 *Food Manufacturing & Economies of Scale: a Modelling Approach* 913  
**Liliana Angeles Martinez, Constantinos Theodoropoulos, Estefania Lopez-Quiroga, Peter J. Fryer and Serafim Bakalis (Liliana Angeles Martinez)**
- 18:10 *Dynamic Programming for Optimal Synthesis of Water Networks in Batch Processes* 919  
**Zhiwei Li and Thokozani Majozi (Zhiwei Li)**
- 18:30 *Biobased Supply Chain Optimisation Model under Uncertainties* 961  
**Anna Panteli, Sara Giarola and Nilay Shah (Anna Panteli)**

**Room D2**

**Chairpersons: Dr. Vicenç Puig and Dr. Filip Logist**

**T4.- Process monitoring and control**

- 16:30 *Efficient Nested Modifier Adaptation for RTO using Lagrangian functions* 1723  
**Tania Rodríguez-Blanco, Daniel Sarabia, Daniel Navia and César de Prada (César de Prada)**
- 16:50 *Resource efficient operation of an evaporator network in the viscose fiber production* 1735  
**Marc Kalliski, Bernhard Voglauer, Gerhard Seyfriedsberger, Christian Jasch, Thomas Röder and Sebastian Engell (Marc Kalliski)**
- 17:10 *Gas Lift Optimization under Uncertainty* 1753  
**Dinesh Krishnamoorthy, Bjarne Foss and Sigurd Skogestad (Dinesh Krishnamoorthy)**
- 17:30 *Economic Optimizing Control for Single-Cell Protein Production in a U-loop Reactor* 1759  
**Andre Drejer, Tobias K. S. Ritschel, Sten Bay Jørgensen and John Bagterp Jørgensen (John Bagterp Jørgensen)**
- 17:50 *Effective Model Adaptation in Iterative RTO* 1717  
**Afaq Ahmad, Weihua Gao and Sebastian Engell (Afaq Ahmad)**

**Room C2**

**Chairpersons: Dr. Petar Varbanov and Dr. Carla Pinheiro**

**T7.- CAPE applications addressing Global Grand Challenges**

- 16:30 *Addressing the Minimum Environmental Impacts of Algal Renewable Diesel Production from a Consequential Perspective* 2605  
**Jian Gong and Fengqi You (Fengqi You)**
- 16:50 *Techno-Economic and Environmental Optimization of Palm-based Biorefineries in the Brazilian Context* 2611  
**Maziar Kermani, Ayse Dilan Celebi, Anna S. Wallerand, Adriano V. Ensinas, Ivan D. Kantor and François Maréchal (Maziar Kermani)**



- 17:10 *Multi-Objective Optimization of a Pressure-Temperature Swing Adsorption Process for Biogas Upgrading* 2629  
**Federico Capra, Matteo Gazzani, Marco Mazzotti, Maurizio Notaro and Emanuele Martelli**  
**(Federico Capra)**
- 17:30 *Production of Fuels from CO<sub>2</sub>-rich Natural Gas using Fischer-Tropsch Synthesis Coupled to Tri-reforming Process* 2659  
**José E. A. Graciano, André D. Carreira, Reinaldo Giudici and Rita M. B. Alves** **(José Eduardo Graciano)**
- 17:50 *Optimal bio-based supply chain with carbon capture and use: an economic and environmental approach* 2665  
**Mar Pérez-Fortes, José Miguel Laínez-Aguirre and Luis Puigjaner** **(Luis Puigjaner)**
- 18:10 *Application of a computer-aided framework for the design of CO<sub>2</sub> capture and utilization processes* 2653  
**Rebecca Frauzem, John M. Woodley and Rafiqul Gani** **(Rebecca Frauzem)**
- 18:30 *On the relevance of thermodynamics to predict the behaviour of inorganics during CO<sub>2</sub> gasification of willow wood* 2671  
**Marwa Said, Laurent Cassayre, Jean-Louis Dirion, Xavier Joulia and Ange Nzihou** **(Laurent Cassayre)**

## 19:00 ... || Cheese and Wine Reception

Hall



## 03, Tuesday

08:00 - 16:30 || Registration

08:00 - 18:00 || Posters

### Poster Hall (P1)

#### T1.- Modeling and Simulation

- P1.25 *Unbiased Selection of Decision Variables for Optimization* 253  
**Mikael Nolin, Niklas Andersson, Bernt Nilsson, Mark Max-Hansen and Oleg Pajalic (Mikael Nolin)**
- P1.26 *Real-time Hybrid Monte Carlo Method for Modelling of 4 Monomer Semi-Batch Emulsion Copolymerization* 259  
**Tomas Chaloupka, Alexandr Zubov and Juraj Kosek (Tomas Chaloupka)**
- P1.27 *Comparison of DLA and RLA Silica-Based Aerogel Structure Modelling Methods* 271  
**Svyatoslav Ivanov, Andrey Tyrtshnikov, Igor Lebedev and Natalia Menshutina (Svyatoslav Ivanov)**
- P1.28 *Model Reduction by Term Elimination and Optimal Selection* 277  
**Brian P. Baillie and George M. Bollas (George Bollas)**
- P1.29 *Realistic Assessment of Parameter Uncertainty in Dynamic Parameter Estimation* 283  
**Mordechai Shacham and Neima Brauner (Mordechai Shacham)**
- P1.30 *Identifiability Analysis and Model Reduction of a Semi-batch Emulsion Polymerization Process Model* 295  
**Preet J. Joy, Adel Mhamdi and Alexander Mitsos (Preet Joy)**
- P1.31 *A Kinetic Study for the Fenton and Photo-Fenton Paracetamol Degradation in a Pilot Plant Reactor* 301  
**Francesca Audino, Leandro Conte, Agustina Schenone, Montserrat Pérez-Moya, Moisés Graells and Orlando Mario Alfano (Francesca Audino)**
- P1.32 *Subspace identification for MIMO systems in the presence of trends and outliers* 307  
**Mikael Manngård, Jari M. Böling and Hannu T. Toivonen (Mikael Manngård)**
- P1.33 *Estimation of Data Uncertainty in the Absence of Repetition Experiments* 313  
**Wei Dai, Selen Cremaschi, Hariprasad J. Subramanib and Haijing Gao (Wei Dai)**
- P1.34 *Experience with large-scale dynamic model validation – application to industrial plant* 325  
**J. Pieter Schmal and Peter J. T. Verheijen (Pieter Schmal)**
- P1.35 *Modelling of the oxy-combustion fluid catalytic cracking units* 331  
**Chao Fu and Rahul Anantharaman (Chao Fu)**
- P1.36 *A Comprehensive Model for the Simulation of Ethylene Decomposition in High-Pressure LDPE Autoclaves* 337  
**Prokopios Pladis, Apostolos Baltas and Costas Kiparissides (Costas Kiparissides)**
- P1.37 *Modeling of a pyrolysis process for the elimination of epoxy resin from embedded nuclear fuels* 343  
**Aziza Chairat, Zhiya Duan, Olivier Fiquet, Carine Ablitzer, Laurent Cassayre, Hugues Vergnes, Pascal Floquet and Xavier Joulia (Zhiya Duan)**
- P1.38 *Process Modeling and Analysis of Manufacturing Pathways for Producing Ethylene and Propylene from Wet Shale Gas and Naphtha* 361  
**Minbo Yang and Fengqi You (Minbo Yang)**
- P1.39 *Flowsheet Simulation of Cobalt–Nickel Separation Using Ionic Liquid Cyphos 101* 373  
**Hongyan Chen and Megan Jobson (Hongyan Chen)**



- P1.40 *Integrated treatment processes for coal-gasification wastewater with high concentration of phenol and ammonia* 379  
**Peizhe Cui, Siyu Yang and Yu Qian (Yu Qian)**
- P1.41 *Technical Feasibility of AG2S<sup>TM</sup> Process Revamping* 385  
**Andrea Bassani, Carlo Pirola, Giulia Bozzano, Eliseo Ranzi and Flavio Manenti (Andrea Bassani)**
- P1.42 *Reverse osmosis for water purification and reuse in the biotechnological industry: Process design, operation and economic guidelines* 391  
**Seyed Soheil Mansouri, Isuru A. Udugama, Aleksandar Mitic, Alexander Rubin, Linnea Rudolfsson and Krist V. Gernaey (Seyed Soheil Mansouri)**
- P1.43 *Distillation Sequence Efficiency (DSE) for Suitable Liquid-Liquid Extraction Solvents: Acetic Acid Extraction with TOA* 397  
**Alexandra Elena Bonet-Ruiz, Rafael Luna Surinyach, Valentin Plesu, Jordi Bonet, Petrica Iancu and Joan Llorens (Alexandra Elena Bonet Ruiz)**
- P1.44 *Process Design for production of 1,3-Butadiene and Methyl Ethyl Ketone from Dehydration of 2,3-Butanediol* 403  
**Yeong-Gak Yoon, Dae-Sung Song and Chul-Jin Lee (Yeong-Gak Yoon)**
- P1.45 *Energy Efficient Hybrid Gas Separation with Ionic Liquids* 421  
**Xinyan Liu, Xiaodong Liang, Rafiqul Gani, Xiangping Zhang and Suojiang Zhang (Xinyan Liu)**

## Poster Hall (P2)

### T2.- Synthesis and Design

- P2.23 *Mitigation of Fouling in Crude Preheat Trains by Simultaneous Dynamic Optimization of Flow Rate and Velocity Distribution* 817  
**Ruonan Liu, Yufei Wang and Xiao Feng (Ruonan Liu)**
- P2.24 *Integration of Bio-refinery Concepts in Oil Refineries* 829  
**Harvey Arellano-Garcia, Elham Ketabchi and Tomas Ramirez Reina (Elham Ketabchi)**
- P2.25 *Model Based Analysis of a Petroleum Refinery Plant with Hydrotreating as a Pre-treatment Unit* 835  
**Mohammad Alkandari, Iqbal M. Mujtaba and Harvey Arellano-Garcia (Mohammad Alkandari)**
- P2.26 *Optimal Design of Refinery Hydrogen Network with Mixed Pattern Configuration* 841  
**Chun Deng, Yeyang Zhou and Xiao Feng (Chun Deng)**
- P2.27 *Integrated Process Design Optimization Accounting for Co-Digestion of Sludge and Municipal Solid Waste* 853  
**Betzabet Morero, Agustín F. Montagna, Enrique Campanella and Diego C. Cafaro (Diego C. Cafaro)**
- P2.29 *Optimal Design of a Wastewater Treatment Plant using Advanced Technologies* 865  
**Vicenç Puig, Juli Romera, Fatiha Nejjari, Joseba Quevedo and Sergi de Campos (Vicenç Puig)**
- P2.30 *Design of a wheat straw supply chain network in Lower Saxony, Germany through optimization* 871  
**Christos Galanopoulos, Angelo Odierna, Diego Barletta and Edwin Zondervan (Christos Galanopoulos)**
- P2.31 *Optimal Design of Poly (3-hydroxybutyrate) Production using alternative Carbon Sources* 877  
**Fernando D. Ramos, Marcelo A. Villar and Maria Soledad Diaz (Maria Soledad Diaz)**
- P2.32 *Superstructural economic optimization of sugarcane bagasse exploitation in an ethanol distillery connected to Rankine cycle, BIGCC system and second generation ethanol process* 889  
**Gabriel C. Fonseca, Caliane B. B. Costa and Antonio J. G. Cruz (Caliane B. B. Costa)**
- P2.33 *Design of desalinated water distribution networks including energy recovery devices* 925  
**Natalia Araya, Luis A. Cisternas, Freddy Lucay and Edelmira D. Gálvez (Edelmira D. Galvez)**





- P2.34 *Process integration for the supercritical production of biodiesel and the production of lignocellulosic bioethanol.* 931  
**Fernando I. Gómez-Castro, María Guadalupe Aldana-González, Carolina Conde-Mejía, Claudia Gutiérrez-Antonio, Araceli G. Romero-Izquierdo and Ricardo Morales-Rodríguez (Fernando I. Gomez-Castro)**
- P2.35 *Optimal Design of Cogeneration Systems Based on Flaring and Venting Streams and Accounting for the Involved Uncertainty* 937  
**Javier Tovar-Facio, Fadwa Eljack, José María Ponce-Ortega and Mahmoud M. El-Halwagi (Jose Maria Ponce-Ortega)**
- P2.36 *A meta-heuristic approach for financial risks management in heat exchanger networks* 955  
**Leandro V. Pavão, Carlos Pozo, Caliane B. B. Costa, Mauro A. S. S. Ravagnani and Laureano Jiménez (Mauro A. S. S. Ravagnani)**
- P2.37 *A Fuzzy Analytic Hierarchy Process Approach for Multi-objective Molecular Design Problem* 967  
**Jecksin Ooi, Michael Angelo B. Promentilla, Raymond R. Tan, Denny Kok Sum Ng and Nishanth G. Chemmangattuvalappil (Jecksin Ooi)**
- P2.38 *The Systematic Screening Methodology for Surfactant Flooding Chemicals in Enhanced Oil Recovery* 991  
**Cholathis Cholpraves, Pattamas Rattanaudom, Uthaiporn Suriyapraphadilok, Ampira Charoensaeng and Rafiqul Gani (Cholathis Cholpraves)**
- P2.39 *Comparison of Tree Based Ensemble Machine Learning Methods for Prediction of Rate Constant of Diels-Alder Reaction* 997  
**Vikrant A. Dev, Shounak Datta, Nishanth G. Chemmangattuvalappil and Mario R. Eden (Vikrant A. Dev)**
- P2.40 *PU foams: Mathematical modelling of morphology development* 1009  
**Juraj Kosek, Pavel Ferkl and Iveta Kršková (Juraj Kosek)**
- P2.42 *Modeling the drug release from ionic and covalent co-cross-linked chitosan hydrogels* 1021  
**Belmiro P. M. Duarte, Maria J. Moura, Maria H. Gil and Maria M. Figueiredo (Belmiro P. M. Duarte)**

## Poster Hall (P5)

### T5.- Integrated/Holistic approaches

- P5.01 *Integrated process and solvent design using COSMO-RS for the production of CO from CO<sub>2</sub> and H<sub>2</sub>* 1765  
**Jan Scheffczyk, Pascal Schäfer, Christian M. Jens, Kai Leonhard and André Bardow (Jan Scheffczyk)**
- P5.02 *Integrated computer-aided framework for chemical product and process application design and optimization for waste heat recovery* 1777  
**Stefano Cignitti, John M. Woodley and Jens Abildskov (Seyed Soheil Mansouri)**
- P5.03 *Design and optimization of Heat Integrated Distillation Column "HIDiC"* 1783  
**Omar Yala, David Rouzineau, Raphaelé Théry-Hétreux and Michel Meyer (Omar Yala)**
- P5.04 *Low Cost Retrofit Methods for Heat Exchanger Networks* 1789  
**Robin Smith and Mary Onome Akpomiemie (Robin Smith)**
- P5.05 *Heat Integration optimization in a Multiproduct Biorefinery* 1801  
**Ségoène Belletante, Ludovic Montastruc, Stéphane Negny, Raphaelé Théry-Hétreux and Serge Domenech (Ludovic Montastruc)**
- P5.06 *Simulation-based analysis for operational decision support on scheduling in sugar crystallization considering quality of molasses and syrup* 1807  
**Kotaro Ouchida, Yosuke Hamada, Tatsuya Okubo and Yasunori Kikuchi (Kotaro Ouchida)**
- P5.07 *Design and optimization of plate heat exchanger networks* 1819  
**Kexin Xu, Robin Smith and Nan Zhang (Kexin Xu)**



- P5.08 Biomass to X: Gasification and Pyrolysis Integrated 1837  
**Andre F Amaral, Giulia Bozzano, Carlo Pirola and Flavio Manenti (Andre F Amaral)**
- P5.09 Retrofit design of hydrogen distribution systems: a practical case study 1843  
**João P. Marques, Henrique A. Matos, Nuno M. C. Oliveira, Clemente P. Nunes, Manuel Prego and Maria A. Guerreiro (João P. Marques)**
- P5.10 Optimization for the flexibility analysis of processes: Application to the acetone-ethanol-butanol producing process 1849  
**Manuel Ramos, Stéphane Gourmelon, Ludovic Montastruc, Stéphane Negny and Serge Domenech (Ludovic Montastruc)**
- P5.11 Ethylene from natural gas via oxidative coupling of methane and cold energy of LNG 1855  
**Arnab Dutta, Chan Wei Chit, Iftekhar A. Karimi and Shamsuzzaman Farooq (Arnab Dutta)**
- P5.12 A Stochastic Approach for Integration of Design and Control under Uncertainty: A Back-off Approach Using Power Series Expansions 1861  
**Mina Rafiei-Shishavan and Luis A. Ricardez-Sandoval (Luis A. Ricardez-Sandoval)**
- P5.14 Integral System to Determine Feasible Regions for Biomass Utilization 1891  
**José Ezequiel Santibañez-Aguilar, Diego Fabián Lozano-García, Francisco J. Lozano and Antonio Flores-Tlacuahuac (Jose Ezequiel Santibañez-Aguilar)**
- P5.15 A Meta-ontology to Design Sustainable Project in a Competitive Stakeholder's Context 1903  
**Anastasia Roth, Vincent Gerbaud, Marianne Boix and Ludovic Montastruc (Anastasia Roth)**
- P5.16 Optimal Coupling of Demand Patterns for Improving the Performance of CHP Systems 1909  
**Luis Fabián Fuentes-Cortés, Víctor M. Zavala, J. Betzabe González-Campos and José María Ponce-Ortega (Jose Maria Ponce-Ortega)**
- P5.17 Systematic Approach to the Extension of Material Exchange in Industrial Symbiosis 1927  
**Ana Somoza-Tornos, Moisès Graells and Antonio Espuña (Ana Somoza-Tornos)**
- P5.18 Design of Circular Economy Plants – The Case of the Textile Waste Biorefinery 1933  
**Foteini Barla, Athanassios Nikolakopoulos and Antonis Kokossis (Foteini Barla)**
- P5.19 Techno-economic analysis of resource recovery technologies for wastewater treatment plants 1945  
**Riccardo Boiocchi, Beatriz Matafome, Carina L. Gargalo, Ana Carvalho and Gürkan Sin (Riccardo Boiocchi)**
- P5.20 Resilience Study Applied in Eco-Industrial Parks 1957  
**Guillermo Valenzuela-Venegas, Francisco Henríquez, Ludovic Montastruc, Marianne Boix and Felipe A. Díaz-Alvarado (Guillermo Valenzuela-Venegas)**
- P5.21 A Natural Gas Monetization Approach with Carbon Dioxide and Excess Heat Integration in Industrial Parks 1963  
**Dhabia Al-Mohannadi, Raid J. Hassiba, Kholoud Abdulaziz and Patrick Linke (Dhabia Al-Mohannadi)**
- P5.22 Economic linear objective function approach for structure optimization of renewables-to-chemicals (R2Chem) networks 1975  
**Dominik Schack, Liisa Rihko-Struckmann and Kai Sundmacher (Dominik Schack)**
- P5.23 Techno-economic Evaluation of an Integrated Microalga Biorefinery Targeting the Co-production of Specialty Chemicals 1981  
**Melina Psycha and Antonis Kokossis (Melina Psycha)**
- P5.24 A design of rural energy system by industrial symbiosis considering availability of regional resources 1987  
**Yuichiro Kanematsu, Kazutake Oosawa, Tatsuya Okubo and Yasunori Kikuchi (Yuichiro Kanematsu)**
- P5.25 A Process Integration Approach to the Optimization of CO<sub>2</sub> Utilization via Tri-Reforming of Methane 1993  
**Mohamed Sufiyan Challiwala, Mohammed Minhaj Ghouri, Debalina Sengupta, Mahmoud M. El-Halwagi and Nimir O. Elbashir (Mohamed Sufiyan Challiwala)**



- P5.26 Cradle-to-gate environmental impact prediction from chemical attributes using mixed-integer programming 1999  
**Raul Calvo-Serrano, María González-Miquel, Stavros Papadokonstantakis and Gonzalo Guillén-Gosálbez (Raul Calvo-Serrano)**
- P5.27 Life Cycle Assessment of vinasse biogas production in sugarcane biorefineries 2017  
**Andreza A Longati, Otávio Cavalett and Antonio J. G. Cruz (Andreza A Longati)**
- P5.28 Addressing decision-making in the process industry using life cycle approach coupled to Linear Programming: A case study on anchovy canning industry in Cantabria Region (Northern Spain) 2023  
**Isabel Garcia-Herrero, Jara Laso, Maria Margallo, Kefah Hjaila, Alba Bala, Cristina Gazulla, Pere Fullana, Ian Vazquez-Rowe, Angel Irabien and Ruben Aldaco (Isabel Garcia-Herrero)**
- P5.29 Modelling pyrolysis process for CFRP recycling in a closed-loop supply chain approach 2029  
**Anaële Lefeuvre, Xavier Yerro, Alan Jean-Marie, Phuong Anh Vo Dong and Catherine Azzaro-Pantel (Phuong Anh Vo Dong)**
- P5.30 Integral Management of Process Plants Systems through their Lifecycle using a Model-Based Engineering Approach 2035  
**Manuel Rodriguez, Ismael Díaz, Julia Bermejo, Ricardo Sanz and Carlos Hernández (Manuel Rodriguez)**

## Poster Hall (P6)

### T6.- Concepts, Methods and Tools

- P6.15 Dynamic Optimization of Batch Processes under Uncertainty via Meta-MultiParametric Approach 2215  
**Ahmed Shokry and Antonio España (Ahmed Shokry)**
- P6.16 A Consistent Methodology Based Parameter Estimation for a Lactic Acid Bacteria Fermentation Model 2221  
**Robert Spann, Christophe Roca, David Kold, Anna Eliasson Lantz, Krist V. Gernaey and Gürkan Sin (Robert Spann)**
- P6.17 Monte Carlo Based Framework to Support HAZOP Study 2233  
**Matej Danko, Jérôme Frutiger, Ľudovít Jelemenský and Gürkan Sin (Matej Danko)**
- P6.18 Probability Density Functions for Droplet Sizing in Aerosol Transport Modelling 2245  
**Pedro I. O. Filho, Dominic B. Potter, Michael J. Powell, Claire J. Carmalt, Panagiota Angeli and Eric S. Fraga (Pedro I. O. Filho)**
- P6.19 Stochastic NMPC/DRTO of Batch Operations: Batch-to-Batch Dynamic Identification of the Optimal Description of Model Uncertainty 2251  
**Francesco Rossi, Flavio Manenti, Guido Buzzi-Ferraris and Gintaras Reklaitis (Francesco Rossi)**
- P6.20 Optimal management of microgrids under uncertainty using scenario reduction 2257  
**Javier Silvente, Lazaros G. Papageorgiou and Vivek Dua (Javier Silvente)**
- P6.21 Design of Experiments Based on Dynamic Real-time Optimization Approach 2269  
**Ryad Bousbia-Salah, François Lesage and Abderrazak Latifi (François Lesage)**
- P6.22 Future of control and operations in the era of industrial internet of things 2275  
**Iiro Harjunoski (Iiro Harjunoski)**
- P6.23 Industry 4.0: Sustainable material handling processes in industrial environments 2281  
**Dimitrios Bechtsis, Naoum Tsolakis, Menippos Vouzas and Dimitrios Vlachos (Dimitrios Bechtsis)**
- P6.24 Know-how Protection and Software Architectures in Industry 4.0 2287  
**Armin Fricke and Jan C. Schöneberger (Armin Fricke)**
- P6.25 The Development of an Online Design Tool for Organic Rankine Cycle 2299  
**Shoulong Dong, Boaz Habib, Howard Zheng, Haiam Abbas, Lei Chen, Holger Heinzl, Matthew Lie, Wei Yu and Brent R. Young (Shoulong Dong)**



- P6.26 *LCSOft – the Life Cycle Assessment Software: New developments and status* 2305  
**Yodsathorn Chavewanmas, Pomthong Malakul and Rafiqul Gani (Yodsathorn Chavewanmas)**
- P6.27 *A Semantic Repository for Model Integration in Biorefining* 2323  
**Edlira Kalemi, Linsey Koo and Franjo Cecelja (Edlira Kalemi)**
- P6.28 *Towards Advanced Enterprise Wide Optimization Based On Explicit Concept-Object Oriented Mathematical Modeling* 2347  
**Edrisi Muñoz, Elisabet Capón-García and José Miguel Láinez-Aguirre (Edrisi Muñoz)**
- P6.29 *Knowledge-Driven Multi-Label Classification of Process Scheduling Problems* 2353  
**Elisabet Capón-García, Edrisi Muñoz, José Miguel Láinez-Aguirre and Konrad Hungerbühler (Elisabet Capon-García)**
- P6.30 *Constraint Identification and Integration Procedures in Multi-Level Hierarchical Systems* 2359  
**Canan Dombayci, Elisabet Capón-García, Edrisi Muñoz and Antonio España (Canan Dombayci)**
- P6.31 *Decision Support based on a Semantically-Enriched Notification Platform at a Process Plant Floor* 2365  
**Chrysovalantou Ziogou, Damiano Arena, Stelios Krinidis, Dimosthenis Ioannidis, Dimitrios Kiritsis, Dimitrios Tzovaras and Spyros Voutetakis (Chrysovalantou Ziogou)**

## Poster Hall (P7)

### T7.- CAPE applications addressing Global Grand Challenges

- P7.28 *Assessing the CO<sub>2</sub> Emissions Reduction from Cement Industry by Carbon Capture Technologies: Conceptual Design, Process Integration and Techno-economic and Environmental Analysis* 2593  
**Calin-Cristian Cormos, Ana-Maria Cormos and Letitia Petrescu (Calin-Cristian Cormos)**
- P7.29 *A low-carbon power generation pathway for China: Scenario analysis with carbon pricing mechanism* 2599  
**Siyuan Chen, Zheng Guo, Pei Liu and Zheng Li (Siyuan Chen)**
- P7.30 *Minimizing CO<sub>2</sub> emissions for syngas production units using Dry Reforming of Methane* 2617  
**Shaik Afzal, Debalina Sengupta, Mahmoud M. El-Halwagi and Nimir Elbashir (Shaik Afzal)**
- P7.31 *Development of a conceptual process for CO<sub>2</sub> capture from flue gases using ionic liquid* 2623  
**Tuan B. H. Nguyen, Stefan G. Reisemann and Edwin Zondervan (Tuan B. H. Nguyen)**
- P7.32 *Analysis of power production and emission reduction through the use of biogas and carbon capture and storage* 2635  
**Ryan Clark, Sara Budinis, Adam Hawkes and Dena McMartin (Ryan Clark)**
- P7.33 *Performance Analysis of Industrial CO<sub>2</sub> Capture from Natural Gas using Diglycolamine* 2641  
**Umer Zahid, Fayez Nasir Al Rowaili, Mohammed Kazeem Ayodeji and Usama Ahmed (Umer Zahid)**
- P7.34 *Modelling, Simulation and Optimisation of an Integrated Two-Stage P/VSA Process for Post-Combustion CO<sub>2</sub> Capture Using Combinations of Adsorbents* 2647  
**George N. Nikolaidis, Eustathios S. Kikkinides and Michael C. Georgiadis (Michael C. Georgiadis)**
- P7.35 *Integrated production planning and water management in the food industry: A cheese production case study* 2677  
**Sai Jishna Pulluru, Renzo Akkerman and Andreas Hottenrott (Sai Jishna Pulluru)**
- P7.36 *Interplant Water Networks Coupled with Two-Stage Treatment and ZLD Options* 2683  
**Sabla Y. Alnouri, Patrick Linke and Mahmoud M. El-Halwagi (Sabla Y. Alnouri)**
- P7.37 *Optimising the total benefit of water resources management in combination with the local energy systems in remote communities taking into account sustainability considerations* 2689  
**Christiana Papapostolou, Emilia Kondili and John K. Kaldellis (Emilia Kondili)**



- P7.38 Optimization of a Distributed Wastewater Treatment Network Considering Lumped Parameters Interrelations 2701  
**Francesca Audino, Sergio Medina-González, Moisès Graells, Montserrat Pérez-Moya, Antonio Espuña and Carlos Alberto Méndez (Francesca Audino)**
- P7.39 Assessment of sustainable wastewater treatment networks design applying LCA 2707  
**Juan I. Padrón-Páez, Ana Carvalho, Oscar Andrés Prado-Rubio and Alicia Román-Martínez (Juan I. Padrón-Páez)**
- P7.40 Optimisation of membrane design parameters of a spiral-wound reverse osmosis module for high rejection of dimethylphenol from wastewater at low energy consumption 2713  
**Mudhar A. Al-Obaidi, Chakib Kara-Zaitri and Iqbal M. Mujtaba (Iqbal M. Mujtaba)**
- P7.41 Towards Sustainable Flux Determination for Dynamic Ultrafiltration through Multivariable System Identification 2719  
**Oscar Andrés Prado-Rubio and Moritz von Stosch (Oscar Andrés Prado-Rubio)**
- P7.42 Combining Forward and Reverse Osmosis for Shale Gas Wastewater Treatment to Minimize Cost and Freshwater Consumption 2725  
**Raquel Salcedo-Díaz, Rubén Ruiz-Femenia, Alba Carrero-Parreño, Viviani C. Onishi, Juan A. Reyes-Labarta and José A. Caballero (Raquel Salcedo Diaz)**
- P7.43 Implementation of linear programming and life cycle approach in an Excel application to determine ecoefficiency 2731  
**Gumersindo Feijoo, Sergio Sanmartin and Maria Teresa Moreira (Maria Teresa Moreira)**
- P7.44 A model for the effect of light on the growth of microalgae in outdoor condition 2737  
**Pooya Darvehei, Parisa A. Bahri and Navid R. Moheimani (Pooya Darvehei)**

## 08:30 - 09:50 || ESCAPE Lectures

### Room D1

Chairpersons: Prof. Michael Fairweather and Prof. Paul Serban Agachi

#### T1.- Modeling and Simulation

- 08:30 Numerical simulation of fixed bed for CO<sub>2</sub> capture in a fossil fuel emission points by Pressure Swing Adsorption System 415  
**Angel Gutierrez-Ortega, Joaquín Menacho, Rafael Gonzalez-Olmos, Rosa Nomen and Julià Sempere (Julià Sempere)**
- 08:50 Mathematical Modelling of Intensified Extraction for Spent Nuclear Fuel Reprocessing 355  
**Davide Bascone, Panagiota Angeli and Eric S. Fraga (Davide Bascone)**
- 09:10 Modelling of Aerogels Structures Using Intelligent System «AeroGen Structure» 469  
**Igor Mitrofanov, Irina Malysheva, Andrey Kolnoochenko and Natalia Menshutina (Igor Mitrofanov)**
- 09:30 Sequential Multi-Scale Modelling Concepts Applied to the Polyurethane Foaming Process 487  
**Sigve Karolius, Heinz A. Preisig and Henrik Rusche (Sigve Karolius)**

### Room C1

Chairpersons: Prof. Emanuele Martelli and Prof. Mario Eden

#### T2.- Synthesis and Design

- 08:30 Computational Analysis of a Two-Phase Continuous-Flow Magnetophoretic Microsystem for Particle Separation from Biological Fluids 1183  
**Jenifer Gómez-Pastora, Ioannis Karampelas, Eugenio Bringas, Edward P. Furlani and Inmaculada Ortiz (Jenifer Gómez-Pastora)**



- 08:50 Dropwise Additive Manufacturing using Particulate Suspensions: Feasible operating space and throughput rates 1207  
**Andrew Radcliffe and Gintaras V. Reklaitis (Andrew Radcliffe)**
- 09:10 Evaluation of an Immiscible Drop Separation System in Micro-channels using CFD 1195  
**Carlos Enrique Llano-Serna, Javier Fontalvo-Alzate and Oscar Andrés Prado-Rubio (Oscar Andrés Prado-Rubio)**
- 09:30 A Fuzzy Programming Approach to Multi-Objective Optimization for Geopolymer Product Design 1015  
**Michael Angelo B. Promentilla, Martin E. Kalaw, Hoc Thang Nguyen, Kathleen B. Aviso and Raymond R. Tan (Michael Angelo B. Promentilla)**

**Room C3**

**Chairpersons: Prof. Costin Sorin Bildea and Prof. Sigurd Skogestad**

**T4.- Process monitoring and control**

- 08:30 Online DEKF for State Estimation in Semi-Batch Free-Radical Polymerization Reactors 1465  
**Santiago D. Salas, Navid Ghadipasha, Wenbo Zhu, Jose A. Romagnoli, T. McAfee and W. F. Reed (Santiago D. Salas)**
- 08:50 Nonlinear Dynamic Process Monitoring: The Case Study of a Multiphase Flow Facility 1495  
**Ruomu Tan, Raphael T. Samuel and Yi Cao (Ruomu Tan)**
- 09:10 Resource efficiency indicators usefulness for decision-making process of operators: refinery hydrogen network case study 1513  
**Anibal Galan, César de Prada, Gloria Gutierrez, Daniel Sarabia, Rafael Gonzalez, Mikel Sola, Sergio Marmol and Carlos Pascual (Anibal Galan)**
- 09:30 A Hierarchical Aggregation Concept for Resource Efficiency in Continuous Production Complexes 1519  
**Benedikt Beisheim, Stefan Krämer and Sebastian Engell (Benedikt Beisheim)**

**Room D2**

**Chairpersons: Dr. Franjo Cecelja and Prof. Tony Kiss**

**T6.- Concepts, Methods and Tools**

- 08:30 Optimal sensor placement strategies for large scale systems 2107  
**Bala Shyamala Balaji and Sridharakumar Narasimhan (Bala Shyamala Balaji)**
- 08:50 Global Identification of Kinetic Parameters via the Extent-based Incremental Approach 2119  
**Diogo Rodrigues, Julien Billeter and Dominique Bonvin (Diogo Rodrigues)**
- 09:10 A center-cut algorithm for solving convex mixed-integer nonlinear programming problems 2131  
**Jan Kronqvist, Andreas Lundell and Tapio Westerlund (Jan Kronqvist)**
- 09:30 SHOT – A global solver for convex MINLP in Wolfram Mathematica 2137  
**Andreas Lundell, Jan Kronqvist and Tapio Westerlund (Andreas Lundell)**

**Room C2**

**Chairpersons: Prof. Fabrizio Bezzo and Prof. Juraj Kosek**

**T7.- CAPE applications addressing Global Grand Challenges**

- 08:30 Powder stickiness in milk drying: uncertainty and sensitivity analysis for process understanding 2743  
**Adrián Ferrari, Soledad Gutiérrez and Gürkan Sin (Adrián Ferrari)**
- 08:50 Waste-Energy-Water systems in sustainable city development using the resilience.io platform 2377  
**Xiaonan Wang, Miao Guo, Koen H. van Dam, Rembrandt H.E.M. Koppelaar, Charalampos Triantafyllidis and Nilay Shah (Xiaonan Wang)**
- 09:10 Pharmaceuticals Removal from Water Effluents by Adsorption in Activated Carbons Using Monte Carlo Simulations 2695  
**Daniel Bahamon and Lourdes F. Vega (Lourdes F. Vega)**



- 09:30 *A computer-aided socio-technical analysis on national and regional energy systems considering local availability of renewable resources* 2485  
**Yasunori Kikuchi, Miwa Nakai, Kazutake Oosawa, Yuichiro Kanematsu, Kotaro Ouchida and Tatsuya Okubo (Yasunori Kikuchi)**

## 10:00 - 11:00 || WCCE Plenary

### Main Auditorium

- 10:00 *Engineering Strategies for a growing world: TR experience*  
**Juan Lladó**  
**Chief Executive Officer**  
**Técnicas Reunidas, Spain**

## 11:00 - 11:45 || Posters / Coffee Break

### Hall

## 11:50 - 13:20 || ESCAPE Keynotes

### Room D7

Chairpersons: Prof. Xavier Joulia and Prof. Sandro Macchietto

#### T5.- Integrated/Holistic approaches

- 11:50 *Screening of Solvents for CO<sub>2</sub> Capture considering Sustainability Criteria via Data Envelopment Analysis* 2011  
**Phantisa Limleamthong, María González-Miquel, Stavros Papadokonstantakis, Athanasios I. Papadopoulos, Panos Seferlis and Gonzalo Guillén-Gosálbez (Gonzalo Guillén-Gosálbez)**
- 12:20 *Life Cycle Optimisation from a Noncooperative Perspective: Game Theory-Based Models and Applications* 1915  
**Jiyao Gao and Fengqi You (Fengqi You)**

#### T2.- Synthesis and Design

- 12:50 *Methodology for biomass blending for the production of power and fuels from biogas* 667  
**Borja Hernández, Erick León and Mariano Martín (Mariano Martín)**

### Room C1

Chairpersons: Prof. Gürkan Sin and Dr. Moisès Graells

#### T1.- Modeling and Simulation

- 11:50 *Graybox Models - New Opportunities for the Optimization of Entire Processes* 97  
**Norbert Asprion, Roger Böttcher, Robert Pack, Marina-Eleni Stavrou, Johannes Höller, Jan Schwientek and Michael Bortz (Norbert Asprion)**

#### T7.- CAPE applications addressing Global Grand Challenges

- 12:10 *Surrogate-based Optimization for Pharmaceutical Manufacturing Processes* 2797  
**Zilong Wang, M. Sebastian Escotet-Espinoza, Ravendra Singh and Marianthi Ierapetritou (Marianthi Ierapetritou)**



- 12:50 *How to Use mechanistic Metabolic Modeling to Ensure High Quality Glycoprotein Production* 2839  
**Alireza Ehsani, Sebastian Niedenfuehr, Thomas Eissing, Swantje Behnken and Andreas Schuppert**  
**(Alireza Ehsani)**

Room C2

Chairpersons: Prof. Ignacio Grossmann and Prof. Antonis Kokossis

## T6.- Concepts, Methods and Tools

- 11:50 *Using Semidefinite Programming to Calculate Bounds on Stochastic Chemical Kinetic Systems at Steady State* 2239  
**Garrett R. Dowdy and Paul I. Barton (Garrett R. Dowdy)**
- 12:20 *Multi-parametric programming based algorithms for the global solution of bi-level mixed-integer linear and quadratic programming problems* 2125  
**Efstratios N. Pistikopoulos and Styliani Avraamidou (Efstratios N. Pistikopoulos)**
- 12:50 *From Ontology to Executable Program Code* 2317  
**Arne Tobias Elve and Heinz A. Preisig (Arne Tobias Elve)**

**13:20 - 14:30 || Lunch**

Catering Area

**13:00 - 14:30 || Comp. & Chem. Engng. - Advisory Board Meeting (by invitation)**

Room: E6 (2<sup>nd</sup> floor)

**14:30 - 15:30 || ESCAPE / WCCE Plenary**

Room C1

Chairperson: Prof. Jiri Jaromir Klemes

- 14:30 *Process Integration: Current Status and Future Challenges* 9  
**Robin Smith**  
**Professor and Director of the Centre for Process Integration**  
**School of Chemical Engineering and Analytical Science**  
**University of Manchester, UK**

**15:30 - 16:25 || Posters / Coffee Break**

Hall

**16:30 - 18:50 || ESCAPE Lectures**

Room C2

Chairpersons: Prof. Iqbal Mujtaba and Prof. Parisa Bahri

## T1.- Modeling and Simulation

- 16:30 *CFD modelling of pulsed sieve plate liquid extraction columns using OPOSPM as a reduced population balance model* 61  
**Samer Alzyod, Menwer Attarakih, Abdelmalek Haseine and Hans-Jörg Bart (Samer Alzyod)**





16:50	Population balance modelling of pulsed packed bed extraction columns using PPB Lab software <b>Menwer Attarakih, Samer Alzyod and Armin Fricke (<u>Menwer Attarakih</u>)</b>	67
17:10	Particle Size Effects on Collision and Agglomeration in Turbulent Channel Flows <b>Tosanbami Ogholaja, Derrick O. Njobuenwu and Michael Fairweather (<u>Tosanbami Ogholaja</u>)</b>	79
17:30	Modelling of Droplet Absorption and Evaporation during Pharmaceutical Tablet Coating <b>Charalampos Christodoulou, Luca Mazzei, Salvador García-Muñoz and Eva Sorensen (<u>Charalampos Christodoulou</u>)</b>	85
17:50	Random porous network generation and 1D mass transfer simulation for gamma-alumina supports <b>Sónia Ferreira, Jan J. Verstraete, Elsa Jolimaitre, Damien Leinekugel-Le-Cocq and Christian Jallut (<u>Sónia Ferreira</u>)</b>	91
18:10	Large Eddy Simulation of Microbubble Transport in Vertical Channel Flows <b>Kenneth S. Asiagbe, Michael Fairweather, Derrick O. Njobuenwu and Marco Colombo (<u>Kenneth S. Asiagbe</u>)</b>	73

**Room C1**

**Chairpersons: Prof. Abderrazak Latifi and Dr. Kathleen Aviso**

**T2.- Synthesis and Design**

16:30	An industrial application of process intensification in the manufacture of dimethyl and diphenyl carbonate <b>Juan Javaloyes-Anton, Sergio Ferrer-Nadal, Ignacio Vic and José A. Caballero (<u>Juan Javaloyes-Anton</u>)</b>	1033
16:50	Hedging Against Uncertain Feedstock Compositions in Shale Gas Processing System Designs with Intensified Equipment Capacities <b>Jian Gong and Fengqi You (<u>Jian Gong</u>)</b>	1051
17:10	Novel Reactive Distillation Processes to produce Diphenyl Carbonate: Multi-Objective Optimization involving Cost and Controllability Criteria <b>Gabriel Contreras-Zarazúa, José Antonio Vazquez-Castillo, Cesar Ramirez-Marquez, Juan Gabriel Segovia-Hernández and Jesus Rafael Alcantara-Avila (<u>Juan Gabriel Segovia-Hernandez</u>)</b>	1069
17:30	Design and Control of Processes for 2-Ethylhexyl Acrylate Production <b>Mihai Daniel Moraru and Costin Sorin Bildea (<u>Mihai Daniel Moraru</u>)</b>	1087
17:50	Innovative design and simulation of a castor oil biorefinery <b>Alexandre Corneliu Dimian, Petrica Iancu, Valentin Plesu, Alexandra-Elena Bonet-Ruiz and Jordi Bonet (<u>Petrica Iancu</u>)</b>	1111
18:10	Model-Based Analysis and Integration of Synthetic Methane Production and Methane Oxidative Coupling <b>Estelle le Sache, Yang Peng, Harvey Arellano-Garcia and Tomas Ramirez Reina (<u>Tomas Ramirez Reina</u>)</b>	1147
18:30	A simplified kinetic and mass transfer modelling of the thermal hydrolysis of vegetable oils <b>Hector Forero-Hernandez, Mark Jones, Bent Sarup, Jens Abildskov, Anker D. Jensen and Gürkan Sin (<u>Hector Forero-Hernandez</u>)</b>	1177

**Room D2**

**Chairpersons: Prof. Marianthi Ierapetritou and Dr. Ludovic Montastruc**

**T5.- Integrated/Holistic approaches**

16:30	Optimal design and operation of water supply chain networks using scenario-based dynamic negotiation and multiple negotiation terms <b>Sergio Medina-González, Fengqi You and Antonio Espuña (<u>Sergio Medina-González</u>)</b>	1921
16:50	Systematic decision making methodology for chemical product design in integrated biorefineries <b>Yen Yi Lai, Kelvin Chu How Yik, Han Peng Hau, Chai Peng Chow and Lik Yin Ng (<u>Lik Yin Ng</u>)</b>	1771



- 17:10 *Integrated thermo-economic design of ORC process, working fluid and equipment using PC-SAFT* 1795  
**Johannes Schilling, Dominik Tillmanns, Matthias Lampe, Madlen Hopp, Joachim Gross and André Bardow (Johannes Schilling)**
- 17:30 *Definition of a Robustness Indicator for Assessment of Heat Exchanger Network Performances* 1813  
**Lucille Payet, Raphaelle Théry-Hétreux, Gilles Hétreux and Pascal Floquet (Lucille Payet)**
- 17:50 *Total Site Integration as a Process Synthesis and Scheduling Tool in Multiple-feedstock Biorefineries* 1825  
**Konstantinos Pyrgakis and Antonis Kokossis (Konstantinos Pyrgakis)**
- 18:10 *An MILP model for simultaneous mass allocation and heat exchange networks design with regeneration units* 1831  
**Sami Ghazouani, Assaad Zoughaib and Solène Le Bourdieu (Sami Ghazouani)**

**Room C4**

**Chairpersons: Prof. Michail Georgiadis and Prof. Stephane Negny**

**T6.- Concepts, Methods and Tools**

- 16:30 *Integrated process performance assessment considering uncertainty in biopharmaceutical manufacturing operations* 2227  
**Gioele Casola, Christian Siegmund, Markus Mattern and Hirokazu Sugiyama (Gioele Casola)**
- 16:50 *Recipe Management based on ISA-88 using Semantic Technologies* 2293  
**Elisabet Capón-García, Edrisi Muñoz, Antonio España and Luis Puigjaner (Elisabet Capón-García)**
- 17:10 *Linking Process Simulation and Automatic 3D Design for Chemical Plants* 2311  
**Sandra Fillinger, Gregor Tolksdorf, Henning Bonart, Erik Esche, Günter Wozny and Jens-Uwe Repke (Sandra Fillinger)**
- 17:30 *Towards an Ontological Backbone for Pharmaceutical Digital Supply Chains* 2329  
**Nikolaos Trokanas and Jagjit Singh Srai (Nikolaos Trokanas)**
- 17:50 *ANSI/ISA 88-95 Standards Based-Approach for Improved Integration of Recipes and Operational Tasks Supported by Knowledge Management* 2335  
**Edrisi Muñoz, Elisabet Capón-García and Luis Puigjaner (Edrisi Muñoz)**
- 18:10 *Integration of CAPE Models and Data for the Domain of Biorefining: InterCAPEmodel Ontology Design* 2341  
**Linsey Koo, Nikolaos Trokanas, Anna Panteli, Edlira Kalemi, Nilay Shah, Madeleine Bussemaker and Franjo Cecelja (Edlira Kalemi)**

**Room C3**

**Chairpersons: Prof. Nuno Oliveira and Dr. Manel Serra**

**T8.- CAPE/PSE Education/Training**

- 16:30 *Implementation of performance indicators for automatic assessment* 2971  
**Laura Marcano, Tiina M. Komulainen and Finn Aakre Haugen (Laura Marcano)**
- 16:50 *Cognitive Behavior Based Framework for Operator Learning: Knowledge and Capability Assessment through Eye Tracking* 2977  
**Laya Das, Babji Srinivasan and Rajagopalan Srinivasan (Laya Das)**
- 17:10 *Recent Evolutions and Trends in the Use of Computer Aided Chemical Engineering for Educational Purposes at the University of Liège* 2941  
**Grégoire Léonard, Sandra Belboom, Dominique Toye, Marie-Noëlle Dumont, Angélique Léonard and Georges Heyen (Dominique Toye)**
- 17:30 *Flipping the Capstone Process Design Course* 2923  
**Daniel R. Lewin and Abigail Barzilai (Daniel R. Lewin)**
- 17:50 *Computer Aided Control Projects as Main Assessment Component of Master's Advanced Control Courses* 2953  
**Carla I. C. Pinheiro and Rui M. Filipe (Carla I. C. Pinheiro)**



- 18:10 *Energy Systems Optimisation: Highlights from an interdisciplinary postgraduate module development* 2965  
***Emilia Kondili and John K. Kaldellis (Emilia Kondili)***
- 18:30 *CAPE in the Chemical Engineering Master's Integrated Programme at IST-ULisboa* 2959  
***Henrique A. Matos, Carla I.C. Pinheiro and Vitor Geraldés (Henrique A. Matos)***

## **20:30 PhD Networking Party**

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**Place to be announced**



## 04, Wednesday

### 08:00 - 16:30 || Registration

Desk

### 08:00 - 18:00 || Posters

#### Poster Hall (P1)

#### T1.- Modeling and Simulation

- P1.50 *Data-Driven Dynamic Modeling of Batch Processes Having Different Initial Conditions and Missing Measurements* 433  
**Ahmed Shokry, Montserrat Pérez-Moya, Moisès Graells and Antonio Espuña (Ahmed Shokry)**
- P1.51 *Measuring the effect on chemical processes due to uncertain input states: Uncertainty-cum-sensitivity analysis using a gPC approach* 439  
**Wahid Ali, Duong Pham Luu Trung, Muhammad Abdul Qyyum, Alam Nawaz and Moonyong Lee (Wahid Ali)**
- P1.52 *Use of Latent Variables to Reduce the Dimension of Surrogate Models* 445  
**Julian Straus and Sigurd Skogestad (Julian Straus)**
- P1.53 *Surrogate Models combined with a Support Vector Machine for the Optimized Design of a Crude Oil Distillation Unit using Genetic Algorithms* 481  
**Dauda Ibrahim, Megan Jobson, Ji Lie and Gonzalo Guillén-Gosálbez (Dauda Ibrahim)**
- P1.54 *Multi-Objective Optimization of Renewable Energy-Driven Desalination Systems* 499  
**Viviani C. Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, Alba Carrero-Parreño, Juan A. Reyes-Labarta and José A. Caballero (Viviani C. Onishi)**
- P1.55 *Modeling Amine Aerosol Growth in CO<sub>2</sub> Capture Absorption Process* 511  
**Jia-Lin Kang, Siao-Han Huang, Guan-Ting Liu, David Shan-Hill Wong and Shi-Shang Jang (Shi-Shang Jang)**
- P1.56 *Modelling of Drying of Biomass Wastes in a Conical Spouted Bed Dryer* 517  
**María J. San José, Sonia Alvarez and Raquel López (María J. San José)**
- P1.57 *Biogas: a Possible New Pathway to Methanol?* 523  
**Giulia Bozzano, Carlo Pirola, Cristina Italiano, Renato Pelosato, Antonio Vita and Flavio Manenti (Cristina Italiano)**
- P1.58 *Material Flow Analysis (MFA) and Life Cycle Assessment Study for Sustainable Management of PVC Wastes in Thailand (Phase III)* 535  
**Wikanda Khomchu, Suriyaphong Nakem, Jirawadee Pipatanatornkul, Seksan Papong, Thanakorn Rodcharoen, Ampira Charoensaeng, Manit Nithitanakul and Pomthong Malakul (Wikanda Khomchu)**
- P1.59 *Model identification, calibration and validation of the aerobic stage in water remediation of a paper mill effluent* 547  
**Fabiola Aguiñaga-Morales, Juan I. Padrón-Páez and Alicia Román-Martínez (Fabiola Aguiñaga-Morales)**
- P1.60 *Modelling and Simulation of Advanced Oxidation Processes: Application to the Treatment of Ciprofloxacin in Aqueous Solution by Ozonation Process* 553  
**María Adelfa Abreu Zamora, Antonio Carlos Silva Costa Teixeira and Galo Antonio Carrillo Le Roux (Galo Antonio Carrillo Le Roux)**



- P1.61 Numerical analysis of hydrogen ventilation in a confined facility with various opening sizes, positions and leak quantities 559  
**Jaewon Lee, Seungsik Cho, Chanho Park, Hyungtae Cho and Il Moon (Jaewon Lee)**
- P1.62 Computational Fluid Dynamics (CFD) Simulation of Fuel Gas and Steam Mixtures to Decrease NOx Emissions of Industrial Burners 565  
**Petrica Iancu, Salvador Vilas-Bonafoux, Jose Manuel Iglesias-Fernandez, Valentin Plesu, Jordi Bonet, Alexandra Elena Bonet-Ruiz and Joan Llorens (Petrica Iancu)**
- P1.63 Multistage Membrane Distillation for the Treatment of Shale Gas Flowback Water: Multi-Objective Optimization under Uncertainty 571  
**Alba Carrero-Parreño, Viviani C. Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, José A. Caballero and Juan A. Reyes-Labarta (Alba Carrero-Parreño)**
- P1.64 Smart software framework for the prediction of accidents consequences in process industries 583  
**Juraj Labovský, Zuzana Labovská, Matej Danko, Ján Janošovský and Ľudovít Jelemenský (Juraj Labovský)**
- P1.65 Using MFM methodology to generate and define major accident scenarios for quantitative risk assessment studies 589  
**Xinsheng Hu, Zongzhi Wu, Morten Lind, Jing Wu, Xinxin Zhang, Jérôme Frutiger and Gürkan Sin (Jing Wu)**

## Poster Hall (P2)

### T2.- Synthesis and Design

- P2.43 Biobutanol Purification by Hybrid Extraction-Divided Wall Column Configurations 1027  
**Massimiliano Errico, Eduardo Sánchez-Ramírez, Juan José Quiroz-Ramírez, Ben-Guang Rong and Juan Gabriel Segovia-Hernández (Massimiliano Errico)**
- P2.44 Modelling and Intensification of Biocatalytic Production of Natural Compounds Performed in Hybrid Systems 1039  
**Ivan Cervenansky, Mario Mihal and Jozef Markos (Ivan Cervenansky)**
- P2.45 Efficient optimization-based design of energy-intensified azeotropic distillation processes 1045  
**Thomas Waltermann, Daniel Münchrath and Mirko Skiborowski (Thomas Waltermann)**
- P2.46 Computational studies on flow maldistribution of Newtonian liquids in periodic packed beds 1057  
**Soumendu Dasgupta and Arnab Atta (Soumendu Dasgupta)**
- P2.47 A study on the periodic operation of an ethanol fermentation process 1063  
**Chi Zhai, Ahmet Palazoglu and Wei Sun (Chi Zhai)**
- P2.48 Design and Control of a Separation Process for Bioethanol Purification by Reactive Distillation 1075  
**Devrim B. Kaymak (Devrim B. Kaymak)**
- P2.49 Development of an intensified Reactive Distillation Process for the Synthesis of Dioxolane Products 1081  
**Arick Castillo-Landero, Arturo Jiménez-Gutiérrez and Rafiqul Gani (Arick Castillo-Landero)**
- P2.50 Retrofitting via Intensification: Application to Formic Acid Process 1093  
**Sergio da Cunha, Gade Pandu Rangaiah and Kus Hidajat (Sergio da Cunha)**
- P2.51 Recovery of succinic acid in fermentation broth via reactive LL extraction: effect of chemical kinetics and solvent choice 1099  
**Benoit Mizzi, Michel Meyer, Laurent Prat, Frédéric Augier and Damien Leinekugel-Le-Cocq (Benoit Mizzi)**
- P2.52 Stability Study of a Hybrid Reactor with Liquid-Liquid Extraction for ABE Production 1105  
**Victor Hugo Grisales Diaz and Gerard Olivar-Tost (Victor Hugo Grisales Diaz)**
- P2.53 Membrane-cryogenic Distillation Hybrid Processes for Cost-effective Argon Production from Air 1117  
**Merve Ceylan, Megan Jobson and Robin Smith (Merve Ceylan)**



- P2.54 Optimal Production of Ethyl Tert-butyl Ether using Pervaporation-based Hybrid Processes through the Analysis of Process Flowsheet 1123  
**Daniel Gorri, Adham Norkobilov and Inmaculada Ortiz (Daniel Gorri)**
- P2.55 Design of a Hybrid Nanofiltration/Electrooxidation Process for the Removal of Perfluorohexanoic Acid (PFHxA) 1129  
**Álvaro Soriano, Daniel Gorri and Ane Urtiaga (Álvaro Soriano)**
- P2.56 Intensification of ethylene glycol production process 1135  
**Apiwit Wisutwattana, Rebecca Frauzem, Uthaiporn Suriyapraphadilok and Rafiqul Gani (Apiwit Wisutwattana)**
- P2.57 Solvent Recycle and Impurity Purge Evaluation for Organosolv Pretreatment Method for Bioethanol Production from Lignocellulosic Biomass 1141  
**André Rodrigues Gurgel da Silva, Massimiliano Errico and Ben-Guang Rong (André Rodrigues Gurgel da Silva)**
- P2.58 Computer-aided design for high efficiency latent heat storage – a case study of a novel domestic solar hot water process 1153  
**Minh Tri Luu, Dia Milani, Mobin Nomvar and Ali Abbas (Ali Abbas)**
- P2.59 General Superstructure Synthesis and Bi-level Solution Strategy for Industrial Heat Pumping 1159  
**Anna S. Wallerand, Maziar Kermani, Ivan D. Kantor and François Maréchal (Anna S. Wallerand)**
- P2.60 Steady-State Plug Flow Reactor Analysis by means of Minimum Entropy 1165  
**David Rosa, Paulo Goes and João Manzi (João Manzi)**
- P2.61 Simultaneous Process Synthesis and Process Intensification using Building Blocks 1171  
**Jianping Li, Salih Emre Demirel and M. M. Faruque Hasan (M. M. Faruque Hasan)**
- P2.62 Computational analysis of facilitated transport in a microfluidic device 1189  
**Arantza Basauri, Jenifer Gómez-Pastora, Marcos Fallanza, Eugenio Bringas and Inmaculada Ortiz (Arantza Basauri)**
- P2.63 Numerical investigation of viscous effect on Taylor bubble formation in co-flow microchannel 1201  
**Somasekhara Goud Sontti and Arnab Atta (Somasekhara Goud Sontti)**
- P2.64 Re-entrant structural evolution using electrically heterogeneous patterned electrode 1213  
**Swarit Dwivedi, Rabibrata Mukherjee and Arnab Atta (Swarit Dwivedi)**
- P2.65 Plant-Wide Design and Control of an Epichlorohydrin Synthesis Process by Reacting Allyl Chloride and Hydrogen Peroxide 1219  
**Chien-Chih Huang, San-Jang Wang, David Shan-Hill Wong and Shi-Shang Jang (Shi-Shang Jang)**
- P2.66 Design and Operability Analysis of Membrane Module based on Volumetric Flexibility 1231  
**Vincentius Surya Kurnia Adi and Rosalia Laxmidewi (Vincentius Surya Kurnia Adi)**
- P2.67 Systematic Methods for Inherently Safer Process Design: Comparison among Inherent Safety Indexes by Dimensionality Reduction 1237  
**Daniel Vázquez, Natalia Quirante, Rubén Ruiz-Femenia, María J. Fernández, Raquel Salcedo-Díaz, M. Francisca Gómez-Rico and José A. Caballero (Daniel Vázquez)**

#### Poster Hall (P4)

#### T4.- Process monitoring and control

- P4.01 EKF-NN based Hybrid Estimator for Ethylene Polymerization Process 1459  
**Wachira Daosud, Mohd Azlan Hussain and Paisan Kittisupakorn (Wachira Daosud)**
- P4.02 Optimising and Predicting Performance of Industrial Filtrations using Process Data 1471  
**Franz D. Böhner, Paloma A. Santacoloma, Jens Abildskov and Jakob K. Huusom (Franz D. Böhner)**
- P4.03 Unscented Kalman Filter. Application of the robust approach to polymerization processes 1477  
**Jhovany Tupaz, Mariano Asteasuain and Mabel Sánchez (Jhovany Tupaz Pantoja)**



P4.04	Comparison of Particle Filter and Extended Kalman Filter Algorithms for Monitoring of Bioprocesses <b>Ines V. Stelzer, Julian Kager and Christoph Herwig (<u>Ines V. Stelzer</u>)</b>	1483
P4.05	A model for subsea oil-water gravity separator to estimate unmeasured disturbances <b>Tamal Das, Christoph Josef Backi and Johannes Jäschke (<u>Tamal Das</u>)</b>	1489
P4.06	Profile-driven Features for Offline Quality Prediction in Batch Processes <b>Ricardo Rendall, Bo Lu, Ivan Castillo, Swee-Teng Chin, Leo H. Chiang and Marco S. Reis (<u>Tiago J. Rato</u>)</b>	1501
P4.07	Optimal Sensor Network Design to Monitor the Energy Performances of a Process Plant <b>Hala Rameh, Cong-Toan Tran, Assaad Zoughaib, Marie-Ann Evans and Jean-Paul Gourelia (<u>Hala Rameh</u>)</b>	1507
P4.08	A robust methodology for the sensor fault detection and classification of systematic observation errors <b>Claudia E. Llanos, Mabel C. Sánchez and Ricardo A. Maronna (<u>Claudia E. Llanos</u>)</b>	1525
P4.09	Smith predictor for slug control with large valve stroke time <b>Henry Tandoh, Yi Cao and Adeola Awoyomi (<u>Henry Tandoh</u>)</b>	1531
P4.10	An efficient and rigorous thermodynamic library and optimal-control of a cryogenic air separation unit <b>Jozsef Gaspar, Tobias K. S. Ritschel and John Bagterp Jørgensen (<u>Jozsef Gaspar</u>)</b>	1543
P4.11	Process control of a heat pump assisted extractive DWC for bioethanol dehydration <b>Iulian Patraşcu and Costin Sorin Bildea (<u>Costin Sorin Bildea</u>)</b>	1549
P4.12	Dynamic simulation of thermal energy storage integrated with small-scale solar power plant and organic Rankine cycle <b>Sittiporn Vongsilodkul and Soorathep Kheawhom (<u>Soorathep Kheawhom</u>)</b>	1561
P4.13	Economic Predictive Control of a Pasteurization Plant using a Linear Parameter Varying Model <b>Fatemeh Karimi Pour, Vicenç Puig and Carlos Ocampo-Martinez (<u>Fatemeh Karimi Pour</u>)</b>	1573
P4.14	Advanced Robust MPC Design of a Heat Exchanger: Modeling and Experiments <b>Juraj Oravec, Monika Bakošová, Daniela Pakšiová, Natália Mikušová and Kinga Batárová (<u>Juraj Oravec</u>)</b>	1585
P4.15	A multi-parametric bi-level optimization strategy for hierarchical model predictive control <b>Styliani Avraamidou and Efstratios N. Pistikopoulos (<u>Styliani Avraamidou</u>)</b>	1591
P4.16	A novel back-up control structure to manage non-routine steam upsets in industrial methanol distillation columns <b>Isuru A. Udugama, Coromina Zander, Seyed Soheil Mansouri, Robert Kirkpatrick, Wei Yu and Brent R. Young (<u>Wei Yu</u>)</b>	1597
P4.17	Identification and Model Predictive Control Design of a Polymer Extrusion Process <b>Ioannis Meintanis, George Halikias, Roberto Giovenco, Andreas Yiotis and Kostas Chrysagis (<u>Ioannis Meintanis</u>)</b>	1609
P4.18	Tuning of PI controllers by Differential Evolution with Tabu List method <b>Cesar Ramirez-Marquez, Erick Yair Miranda-Galindo, Juan Gabriel Segovia-Hernández and Salvador Hernández (<u>Juan Gabriel Segovia-Hernandez</u>)</b>	1633
P4.19	Set point tracking of a biogas plant coupled to a methanation reactor <b>Andreas Himmel, Sebastian Sager and Kai Sundmacher (<u>Andreas Himmel</u>)</b>	1645
P4.21	Sliding Dynamic Data Window: Improving Properties of the Incremental Learning Methods <b>Mohammad Hamed Ardakani, Gerard Escudero, Moisés Graells and Antonio Espuña (<u>Mohammad Hamed Ardakani</u>)</b>	1663
P4.22	Process Fault Isolation via Bayesian Lasso-based Reconstruction Analysis <b>Zhengbing Yan and Yuan Yao (<u>Yuan Yao</u>)</b>	1669



- P4.23 Improved Fault Diagnosis in Online Process Monitoring of Complex Networked Processes: a Data-Driven Approach 1681  
**Tiago J. Rato and Marco S. Reis (Tiago J. Rato)**
- P4.24 Root cause diagnosis of disturbances propagation paths by using improved convergent cross mapping 1693  
**Feifan Cheng and Jinsong Zhao (Feifan Cheng)**
- P4.25 Actuator and Sensor Fault Tolerant Control of a Crude Distillation Unit 1705  
**Sulaiman A. Lawal and Jie Zhang (Sulaiman A. Lawal)**
- P4.26 Comparison of regression data selection strategies for quadratic approximation in RTO 1711  
**Simon Wenzel, Vassilios Yfantis and Weihua Gao (Simon Wenzel)**
- P4.27 Modifier-Adaptation Based on Transient Measurements Applied to a Laboratory-Scale Flotation Column 1729  
**Daniel Navia, Antonio Puen, Luis Bergh, Tania Rodríguez-Blanco and César de Prada (Daniel Navia)**
- P4.28 Dynamic Real-time Optimization of a Batch Polymerization Process 1741  
**Ryad Bousbia-Salah, François Lesage, Guo-Hua Hu and Abderrazak Latifi (Ryad Bousbia-Salah)**
- P4.29 Stochastic Approximation in Online Steady State Optimization Under Noisy Measurements 1747  
**Reinaldo Hernández and Sebastian Engell (Reinaldo Hernandez)**

## Poster Hall (P7)

### T7.- CAPE applications addressing Global Grand Challenges

- P7.45 Performance of classical and physiologically-based PK-PD modelling for prediction of remifentanyl hemodynamic effects 2755  
**Adriana Savoca, Roberto Andrea Abbiati and Davide Manca (Davide Manca)**
- P7.46 Developing QSPR for Predicting DNA Drug Binding Affinity of 9-Anilinoacridine Derivatives Using Correlation-Based Adaptive LASSO Algorithm 2767  
**Shounak Datta, Vikrant A. Dev and Mario R. Eden (Shounak Datta)**
- P7.48 [ModLife] Modeling stability of double emulsions 493  
**Behnam Khadem and Nida Sheibat-Othman (Behnam Khadem)**
- P7.49 [ModLife] Multi-scale modelling of solute partition equilibria of micelle-water and microemulsion-water systems using molecular dynamics and COSMOtherm 2773  
**Mattia Turchi, Guoping Lian, Qiong Cai, Ian Wood, Jeremy Rabone and Massimo Noro (Mattia Turchi)**
- P7.50 [ModLife] Multi-scale Modeling Approach for Design and Optimization of Oleochemical Processes 1885  
**Mark Jones, Hector Forero-Hernandez, Bent Sarup and Gürkan Sin (Mark Jones)**
- P7.51 [ModLife] Methodology for Plantwide Design and Optimization of Wastewater Treatment Plants 859  
**Johanna Maria Dragan, Alexandr Zubov and Gürkan Sin (Johanna Maria Dragan)**
- P7.52 [ModLife] Uncertainty and Sensitivity Analysis for an Ibuprofen Synthesis Model Based on Hoechst Path 163  
**Frederico Montes, Krist V. Gernaey and Gürkan Sin (Frederico Montes)**
- P7.53 Process systems engineering approaches for drug product manufacturing: from tablets to injectables 2785  
**Hirokazu Sugiyama, Kensaku Matsunami and Keisho Yabuta (Hirokazu Sugiyama)**
- P7.54 A multi-period model for the optimization of the products and information flows in a healthcare system 2809  
**M. Celeste Kees, M. Susana Moreno and J. Alberto Bandoni (M. Celeste Kees)**
- P7.55 Multi-stage population balance model to understand the dynamics of fed-batch CHO cell culture 2821  
**Sakhr Alhuthali, Sarah Fadda, Cher H. Goey and Cleo Kontoravdi (Sakhr Alhuthali)**





P7.56	An Efficient Experimental Design Strategy for Modelling and Characterization of Processes <b>Tannaz Tajsoleiman, Daria Semenova, Ana C. Fernandes, Jakob Kjøbsted Huusom, Krist V. Gernaey and Ulrich Krühne (Tannaz Tajsoleiman)</b>	2827
P7.57	Kinetic Modelling and Scaled-up Experimental Studies of Microalgal Fuels and Chemicals Production <b>Mesut Bekirogullari, Jon K. Pittman and Constantinos Theodoropoulos (Constantinos Theodoropoulos)</b>	2833
P7.58	Modelling of the imperfect mixing in a hybrid exothermic chemical reactor with simulated heat of reaction <b>Piotr Skupin, Mieczyslaw Metzger, Piotr Laszczyk and Malgorzata Niedzwiedz (Piotr Skupin)</b>	2845
P7.59	Metabolic Network design of <i>Synechocystis</i> sp. PCC 6803 to obtain bioethanol under autotrophic conditions <b>Romina Lasry Testa, Claudio Delpino, Vanina Estrada and Maria Soledad Diaz (Maria Soledad Diaz)</b>	2857
P7.60	Transesterification of Castor Oil Catalyzed by Liquid Enzymes: Optimization of Reaction Conditions <b>Thalles Allan Andrade, Massimiliano Errico and Knud Villy Christensen (Thalles Allan Andrade)</b>	2863
P7.61	Experimental Work Towards the Improvement of a Kinetic Model for Acetone-Butanol-Ethanol Pathway <b>Asal Rahimsalehi, Claudio Avignone-Rossa and Harvey Arellano-Garcia (Harvey Arellano-Garcia)</b>	2875
P7.62	Modeling Biodiesel Production and Purification – Towards a Predictive Tool <b>Lourdes F. Vega, Felix Llovel, J. Torné, S. V. D. Freitas, Mariana B. Oliveira and Joao A. P. Coutinho (Lourdes F. Vega)</b>	2881
P7.63	Attainable Region for Biobutanol Production <b>Cansu Birgen, Heinz A. Preisig, Alexander Wentzel, Sidsel Markussen and Bernd Wittgens (Cansu Birgen)</b>	2893
P7.64	Heat integration for the production process of 2G bioethanol from wheat straw <b>Moises Gonzalez-Contreras, Arturo Sanchez and Teresa Lopez-Arenas (Moises Gonzalez-Contreras)</b>	2917

## 08:30 - 09:50 || ESCAPE Lectures

Room C2

Chairpersons: Prof. Heinz A Preisig and Dr. Norbert Asprion

### T1.- Modeling and Simulation

08:30	Physics-Based Surrogate Models for Optimal Control of a CO <sub>2</sub> Methanation Reactor <b>Karsten Hans Georg Rätze, Jens Bremer, Lorenz T. Biegler and Kai Sundmacher (Karsten Hans Georg Rätze)</b>	127
08:50	Fouling Modelling in Crude Oil Preheat Systems <b>José Loyola-Fuentes, Robin Smith and Megan Jobson (Jose Loyola-Fuentes)</b>	409
09:10	Development and Optimization of a Single Column Analog Model for a Multi-Column Counter-Current Solvent Gradient Purification Process <b>Anton Sellberg, Niklas Andersson, Anders Holmqvist and Bernt Nilsson (Anton Sellberg)</b>	187
09:30	Crystallization of Calcium Carbonate and Magnesium Hydroxide in the Heat Exchangers of Once-through Multistage Flash Process Desalination <b>Salih Alsadaie and Iqbal M. Mujtaba (Iqbal M. Mujtaba)</b>	349



**Room C5**

**Chairpersons: Prof. Shinji Hasebe and Dr. Gabriela Henning**

**T2.- Synthesis and Design**

- 08:30 *A Target Oriented Robust Optimization Model for Selection of Engineering Project Portfolio under Uncertainty* 949  
**Kathleen B. Aviso, Charlle L. Sy and Raymond R. Tan (Kathleen B. Aviso)**
- 08:50 *Robust Design of Chemical Processes Based on a One-Shot Sparse Polynomial Chaos Expansion Concept* 613  
**Xiangzhong Xie, René Schenkendorf and Ulrike Krewer (Xiangzhong Xie)**
- 09:10 *An Optimisation-based Framework for Simultaneous Process Synthesis and Heat Integration* 619  
**Qingyuan Kong and Nilay Shah (Qingyuan Kong)**
- 09:30 *Process Flow-Sheet Synthesis: Systems-Level Design applied to Synthetic Crude Production* 643  
**James Alistair Fox, Diane Hildebrandt, David Glasser and Bilal Patel (James Alistair Fox)**

**Room C3**

**Chairpersons: Prof. Sebastian Engell and Dr. Daniel Sarabia**

**T4.- Process monitoring and control**

- 08:30 *Robust model-based design of experiments for guaranteed parameter estimation* 1639  
**Anwesh Reddy Gottu Mukkula and Radoslav Paulen (Radoslav Paulen)**
- 08:50 *Enhanced global self-optimizing control* 1651  
**Yi Cao and Lingjian Ye (Yi Cao)**
- 09:10 *Effect of Fouling on Control and Energy Recovery in an Industrial CDU Column* 1555  
**Nicholas Seegulam, Francesco Coletti and Sandro Macchietto (Sandro Macchietto)**
- 09:30 *Rethinking Boilers Control* 1537  
**Vanessa Conz, Guilherme de Mello Kich, Rafael Lopes de Oliveira, Renata Beck Hormazabal and Adriano da Silva Vieira (Vanessa Conz)**

**Room C4**

**Chairpersons: Prof. Emilia Kondili and Dr. Pedro Castro**

**T3.- Planning and Scheduling**

- 08:30 *Mixed-Integer Models for Simultaneous Optimization of Inventory Policies and Supply Chain Planning* 1255  
**Braulio Brunaud, José Miguel Laínez-Aguirre, Jose M. Pinto and Ignacio E. Grossmann (Braulio Brunaud)**
- 08:50 *Closed loop integration of planning, scheduling and control via exact multi-parametric nonlinear programming* 1273  
**Vassilis M. Charitopoulos, Vivek Dua and Lazaros G. Papageorgiou (Vassilis M. Charitopoulos)**
- 09:10 *Dynamic Optimization and Control Strategy for the Planning of a Waste Management System involving Multiple Cities* 1291  
**José Ezequiel Santibañez-Aguilar, Antonio Flores-Tlacuahuac, Martín Rivera-Toledo and José María Ponce-Ortega (Jose Ezequiel Santibañez-Aguilar)**
- 09:30 *A Hybrid Slot-Based/General Precedence Approach for Planning Crude Oil Supplies* 1321  
**Pedro C. Pautasso, Vanina G. Cafaro, Jaime Cerdá and Diego C. Cafaro (Diego C. Cafaro)**



**Room D2**

**Chairpersons: Prof. Laureano Jiménez Esteller and Dr. Kamal Kuriyan**

**T7.- CAPE applications addressing Global Grand Challenges**

- 08:30 *Power Generation Expansion Considering Endogenous Technology Cost Learning* 2401  
**Clara F. Heuberger, Edward S. Rubin, Iain Staffell, Nilay Shah and Niall Mac Dowell (Clara F. Heuberger)**
- 08:50 *A general superstructure for the optimal synthesis and design of power and inverse Rankine cycles* 2407  
**Cristina Elsidó, Alberto Mian, François Maréchal and Emanuele Martelli (Cristina Elsidó)**
- 09:10 *Optimal design and operation of A-frame systems for solar power plants* 2449  
**José Antonio Luceño and Mariano Martín (Mariano Martín)**
- 09:30 *Economic optimization of integrated lignocellulosic biorefinery* 2503  
**Payala Venkat Vikash and Yogendra Shastri (Yogendra Shastri)**

**10:00 - 11:00 || WCCE Plenary**

**Main Auditorium**

- 10:00 *Solving Global Energy Issues*  
**Philippe A. Tanguy**  
*Vice President R&D Partnerships*  
*Total, France*

**11:00 - 11:45 || Posters / Coffee Break**

**Hall**

**11:50 - 13:10 || ESCAPE Lectures**

**Room C2**

**Chairpersons: Prof. Ian Cameron and Prof. Brent Young**

**T1.- Modeling and Simulation**

- 11:50 *Efficient Surrogate Model Development: Optimum Model Form Based on Input Function Characteristics* 457  
**Sarah E. Davis, Selen Cremaschi and Mario R. Eden (Sarah Davis)**
- 12:10 *Mixed-Integer MultiParametric Approach based on Machine Learning Techniques* 451  
**Ahmed Shokry, Sergio Medina-González and Antonio Espuña (Ahmed Shokry)**
- 12:30 *Automatic Generation of Simulation Code for Embedding Custom Unit Operations in CAPE Software* 463  
**Gregor Tolksdorf, Erik Esche, Günter Wozny and Jens-Uwe Repke (Gregor Tolksdorf)**
- 12:50 *Enhanced Procedure for Simultaneous Synthesis of an entire Total Site* 427  
**Andreja Nemet and Zdravko Kravanja (Andreja Nemet)**

**Room C5**

**Chairpersons: Dr. Petrica Iancu and Dr. Giulia Bozzano**

**T2.- Synthesis and Design**

- 11:50 *Computational chemical product design problems under property uncertainties* 973  
**Jérôme Frutiger, Stefano Cignitti, Jens Abildskov, John M. Woodley and Gürkan Sin (Jerome Frutiger)**



- 12:10 *The Chemical Product Simulator – ProCAPD* 979  
**Sawitree Kalakul, Mario R. Eden and Rafiqul Gani (Sawitree Kalakul)**
- 12:30 *An Integrated Methodology for Emulsified Cosmetic Product Formulation Using Integer Programming with Logical Constraints* 985  
**Javier A. Arrieta-Escobar, Fernando P. Bernardo, Alvaro Orjuela, Mauricio Camargo and Laure Morel (Javier A. Arrieta-Escobar)**
- 12:50 *gSAFT: Advanced physical property prediction for process modelling* 1003  
**Thomas Lafitte, Vasileios Papaioannou, Simon Dufal and Constantinos C. Pantelides (Vasileios Papaioannou)**

**Room C3**

**Chairpersons: Prof. Constantinos Theodoropoulos and Dr. Gerard Escudero**

**T4.- Process monitoring and control**

- 11:50 *An Efficient Polynomial Chaos Expansion Strategy for Active Fault Identification of Chemical Processes* 1675  
**René Schenkendorf, Xiangzhong Xie and Ulrike Krewer (René Schenkendorf)**
- 12:10 *Active Fault Detection and Identification using Transient Data* 1687  
**Kyle A. Palmer and George M. Bollas (George M. Bollas)**
- 12:30 *Use of Discrete-Event Dynamic Systems for HAZOP Analysis* 1699  
**Mandar N. Thombre and Heinz A. Preisig (Mandar N. Thombre)**
- 12:50 *Toward Online Explore of Concept Drift for Fault Detection of Chemical Processes* 1657  
**Mohammad Hamed Ardakani, Mahdiah Askarian, Gerard Escudero, Moisès Graells and Antonio Espuña (Mahdiah Askarian)**

**Room D2**

**Chairpersons: Prof. Francois Marechal and Dr. Elisabet Capon-Garcia**

**T7.- CAPE applications addressing Global Grand Challenges**

- 11:50 *Model-Based Optimization of Battery Energy Storage Systems* 2563  
**Leonardo K. K. Maia, Zeynep Güven, Fabio La Mantia and Edwin Zondervan (Leonardo K. K. Maia)**
- 12:10 *Integration of Decision Tools in EMS* 2467  
**Fernán Serralunga, Juan P. Ruiz, Diego Ruiz and Carlos Ruiz (Diego Ruiz)**
- 12:30 *A systems engineering framework for application-dependent identification and design of electrochemical energy conversion systems* 2587  
**Deepa Elizabeth Eapen and Raghunathan Rengaswamy (Deepa Elizabeth Eapen)**

**Room C4**

**Chairpersons: Prof. Henrique Matos and Prof. Daniel Lewin**

**T8.- CAPE/PSE Education/Training**

- 11:50 **EURECHA Student Contest Awards 2017**
- 12:00 *Support of Education in Process Simulation and Optimization via Language Independent Modelling and Versatile Code Generation* 2929  
**Erik Esche, Gregor Tolksdorf, Sandra Fillinger, Henning Bonart, Günter Wozny and Jens-Uwe Repke (Erik Esche)**
- 12:30 *Discrete optimization in the chemical engineering curriculum* 2947  
**Fernando P. Bernardo and Nuno M. C. Oliveira (Fernando P. Bernardo)**
- 12:50 *Web-based Operator Training System* 2935  
**Manel Serra, Erika Franco, Luis Rumi, José María Ferrer and José María Nougues (Manel Serra)**



## 13:10 - 14:30 || Lunch

### Catering Area

## 14:30 - 15:30 || WCCE Plenary

### Main Auditorium

14:30 *Challenges and Opportunities for Chemical Engineering in an Emerging Solar Economy*

**Rakesh Agrawal** (P.V. Dankwerts Memorial Lecture)

**Winthrop E. Stone Distinguished Professor**

**School of Chemical Engineering**

**Purdue University, USA.**

## 15:30 - 16:25 || Posters / Coffee Break

### Hall

## 16:30 - 18:10 || ESCAPE Lectures

### Room C2

Chairpersons: Prof. Harvey Arellano-Garcia and Dr. Alexandra Elena Bonet Ruiz

#### T1.- Modeling and Simulation

- 16:30 *Introducing Green GDP as an Objective to Account for Changes in Global Ecosystem Services Due to Biofuel Production* 505  
**Daniel J. Garcia and Fengqi You (Daniel J. Garcia)**
- 16:50 *Carbon Arbitrage with Stationary Batteries in the City of London* 529  
**Mauricio Riveros, Miao Guo, Koen H. van Dam, Gonzalo Bustos and Nigel Brandon (Mauricio Riveros)**
- 17:10 *Sustainable supply chain design and planning: the importance of life cycle scope definition* 541  
**Bruna Mota, Ana Carvalho, Maria Isabel Gomes and Ana Paula Barbosa-Póvoa (Ana Paula Barbosa-Póvoa)**
- 17:30 *Sustainability Assessment of an Integrated Economic-Ecologic-Social Model Under Time-Dependent Uncertainties* 577  
**Pablo Tenoch Rodriguez-Gonzalez, Vicente Rico-Ramirez, Ramiro Rico-Martinez and Urmila M. Diwekar (Pablo Tenoch Rodríguez-González)**

### Room C5

Chairpersons: Prof. Thokozani Majozi and Dr. Igor Plazl

#### T2.- Synthesis and Design

- 16:30 *Computer Aided Synthesis of Innovative Processes: Renewable Adipic Acid Production* 709  
**Alessandro Rosengart, Maria-Ona Bertran, Flavio Manenti, Attilio Citterio, John M. Woodley and Rafiqul Gani (Alessandro Rosengart)**
- 16:50 *Optimization-based early phase design of a homogeneously catalysed process in a thermomorphic solvent system* 715  
**Francesco Benski, Corina Nentwich and Sebastian Engell (Corina Nentwich)**
- 17:10 *Production Zone Method: a New Non-ideal Shortcut Method for Distillation Column Design* 745  
**Guillaume Worms, Michel Meyer, David Rouzineau and Mathias Brehelin (Guillaume Worms)**



- 17:30 *Distillation Sequence Efficiency (DSE) Applied to Trains of Columns with Recycle Streams* 751  
**Jordi Bonet, Alex Parra Paz, Alexandra Elena Bonet-Ruiz, Valentin Plesu, Petrica Iancu and Joan Llorens (Jordi Bonet)**
- 17:50 *Multi-objective Optimization of a Methanol Synthesis Process Superstructure with Two-step Carbon Dioxide Consumption* 721  
**Juan D. Medrano, Rubén Ruiz-Femenia and José A. Caballero (Juan D. Medrano)**

**Room C3**

**Chairpersons: Prof. Luis Puigjaner and Prof. Carlos Alberto Mendez**

**T3.- Planning and Scheduling**

- 16:30 *Hierarchical Waste Incineration Planning and Scheduling System for Industrial Operation Support* 1327  
**Matteo L. Abaecherli, Daniel Santos González, Samuel Perren, Elisabet Capón-García, Andrej Szijarto and Konrad Hungerbühler (Matteo L. Abaecherli)**
- 16:50 *Stochastic Modeling Approach for Downstream Oil Supply Chain* 1339  
**Camilo Lima, Susana Relvas and Ana Paula Barbosa-Póvoa (Camilo Lima)**
- 17:10 *Hedging Against Uncertainty in Process Planning: A Data-Driven Adaptive Nested Robust Optimization Approach* 1345  
**Chao Ning and Fengqi You (Chao Ning)**
- 17:30 *Water Security and Clean Energy, Co-benefits of an Integrated Water and Energy Management* 1363  
**Negar Vakilifard, Parisa A. Bahri, Martin Anda and Goen Ho (Negar Vakilifard)**
- 17:50 *New Continuous-Time Scheduling Formulation for Multiproduct Pipelines* 1381  
**Pedro M. Castro and Hossein Mostafaei (Pedro M. Castro)**

**Room C4**

**Chairpersons: Prof. Pascal Floquet and Prof. Hirokazu Sugiyama**

**T6.- Concepts, Methods and Tools**

- 16:30 *Bayesian Multi-Objective Optimisation of Neotissue Growth in a Perfusion Bioreactor Set-Up* 2155  
**Simon Olofsson, Mohammad Mehrian, Liesbet Geris, Roberto Calandra, Marc Peter Deisenroth and Ruth Misener (Simon Olofsson)**
- 16:50 *Dynamic Optimization of the Production of Monoclonal Antibodies in Semi-batch Operation* 2161  
**Chrysoula Dimitra Kappatou, Adel Mhamdi, Ana Quiroga Campano, Athanasios Mantalaris and Alexander Mitsos (Chrysoula Dimitra Kappatou)**
- 17:10 *Investigating practical aspects of the exergy based multi-objective optimization of chemical processes* 2173  
**Carlos Andre Muñoz, Dries Telen, Philippe Nimmegeers, Lorenzo Cabianca, Filip Logist and Jan Van Impe (Carlos Andre Muñoz)**
- 17:30 *Solving Dynamic Constraint Trajectory Optimization Problems by Applying the Concept of Pareto Frontiers* 2197  
**Jan C. Schöneberger and Armin Fricke (Jan C. Schöneberger)**
- 17:50 *A Systematic Approach for the Optimal Design of an Off-Grid Polygeneration System using Fuzzy Linear Programming Model* 2191  
**Aristotle T. Ubando, Isidro Antonio Marfori III, Alvin B. Culaba, Jonathan R. Dungca, Michael Angelo B. Pomentilla, Kathleen B. Aviso and Raymond R. Tan (Aristotle T. Ubando)**



Room D2

Chairpersons: Prof. Zdravko Kravanja and Prof. Dominique Toye

### T7.- CAPE applications addressing Global Grand Challenges

- 16:30 *Model-assisted operational design of bacterial PHA-production processes: the obstacle of heterogeneity inducing modules* 2887  
**Christos Chatzidoukas, Aristidis Kondylidis and Dimitrios Meimaroglou (Christos Chatzidoukas)**
- 16:50 *Optimisation of microalgal starch formation for the biochemical production of biobutanol* 2899  
**Gonzalo M. Figueroa-Torres, Jon K. Pittman and Constantinos Theodoropoulos (Gonzalo M. Figueroa Torres)**
- 17:10 *Uncertainty & Sensitivity Analysis of Economic Assessment of Lactic Acid Production from Crude Glycerol – Impact of Price Correlations* 2911  
**Carina L. Gargalo, Ana Carvalho, Krist V. Gernaey and Gürkan Sin (Gürkan Sin)**

### 17:30 ... || Cheese and Wine Reception

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Hall

### 20:30 ... || Gala Dinner

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[Maritime Museum - Drassanes Reials \(link\)](#)



## 05, Thursday

### 08:00 - 12:30 || Registration

Desk

### 08:30 - 09:50 || ESCAPE Lectures

Room C2

Chairpersons: Prof. Oscar Andrés Prado-Rubio and Prof. Christian Jallut

#### T1.- Modeling and Simulation

- 08:30 *Investigation of Hydrodynamic Behaviour in random packing using CFD simulation* 13  
**Jia-Lin Kang, Wei-Fu Chen, Ya-Cih Ciou, David Shan-Hill Wong and Shi-Shang Jang (Jia-Lin Kang)**
- 08:50 *CFD Analysis of Liquid-Liquid Extraction Pulsed Sieve-Plate Extraction Columns* 19  
**Zinedine Khatir, Bruce C. Hanson, Michael Fairweather and Peter J. Heggs (Michael Fairweather)**
- 09:10 *CFD simulation of sieve tray hydraulics using the lattice Boltzmann method* 37  
**Noelia Llorente-Remartínez and Santos Galán (Santos Galán)**
- 09:30 *Numerical Simulation of Two-phase Flow in Representative Elements of Structured Packings* 2089  
**Alexander Olenberg and Eugeny Y. Kenig (Alexander Olenberg)**

Room C5

Chairpersons: Prof. Costas Kiparissides and Prof. Luis Cisternas

#### T2.- Synthesis and Design

- 08:30 *A Dual Methodology for Synthesis of Woody Biomass to Liquid (BtL) Thermochemical Conversion Routes and Bio-oil Upgrading* 679  
**Paola Ibarra-Gonzalez, Carlo Edgar Torres-Ortega and Ben-Guang Rong (Paola Ibarra-Gonzalez)**
- 08:50 *Bio-conversion targeting using a model-based systems approach* 685  
**Georgios P. Panayiotou and Antonis Kokossis (Georgios P. Panayiotou)**
- 09:10 *Simultaneous Optimization of Cooler Network, Pump Network, and Cooling Tower* 763  
**Jiaze Ma, Yufei Wang and Xiao Feng (Jiaze Ma)**
- 09:30 *Locating Heat Exchangers in an EIP-wide Heat Integration Network* 793  
**Sajitha K. Nair, Melvin Soon and Iftekhar A. Karimi (Sajitha K. Nair)**

Room C3

Chairpersons: Dr. Radoslav Paulen and Dr. Maria Soledad Diaz

#### T4.- Process monitoring and control

- 08:30 *Expectation constrained stochastic nonlinear model predictive control of a batch bioreactor* 1621  
**Eric Bradford and Lars Imsland (Eric Bradford)**
- 08:50 *Modeling and nonlinear MPC of a dividing-wall column for separation of Benzene-Toluene-p-Xylene: a simulation case study* 1615  
**João R. Leal, Andrey Romanenko and Lino O. Santos (João R. Leal)**
- 09:10 *Wastewater treatment plants operation optimization using economic dynamic real time optimization strategies* 1567  
**Silvana Revollar, Pastora Vega, Ramon Vilanova and Mario Francisco (Silvana Revollar)**
- 09:30 *Economic Model Predictive Control of Aeration Systems in a Full Scale Biological Wastewater Treatment Plant* 1579  
**Fatiha Nejjari, Vicenç Puig, Joseba Quevedo, Josep Pascual and S. de Campos (Vicenç Puig)**





**Room C4**

**Chairpersons: Prof. David Bogle and Prof. José A. Caballero**

**T5.- Integrated/Holistic approaches**

- 08:30 An MILP model for the simultaneous design of mass and heat networks of a collaborative eco-industrial park 1939  
**Sami Ghazouani, Assaad Zoughaib and Solène Le Bourdieu (Sami Ghazouani)**
- 08:50 Benefits analysis of optimal design of eco-industrial parks through life cycle indicators 1951  
**Marianne Boix, Ludovic Montastruc, Manuel Ramos, Olivier Gentilhomme and Serge Domenech (Serge Domenech)**
- 09:10 A Hybrid Methodology for Combined Interplant Heat, Water, and Power Integration 1969  
**Maziar Kermani, Anna S. Wallerand, Ivan D. Kantor and François Maréchal (Maziar Kermani)**
- 09:30 Optimal Global Land Use, Cultivation, Transportation, and Production Strategies to Minimise Life Cycle Greenhouse Gas Emissions of Ethanol 2005  
**Daniel J. Garcia and Fengqi You (Daniel J. Garcia)**

**Room D2**

**Chairpersons: Dr. Cristhian Almeida-Rivera and Dr. Giorgos Kopanos**

**T7.- CAPE applications addressing Global Grand Challenges**

- 08:30 A Green Desuperheater for an Energetic Efficient Alternative to the Decompression Valve in Supercritical Water Hydrolysis Process. CFD Simulation. 2905  
**Luis Vaquerizo and María José Cocero (Luis Vaquerizo)**
- 08:50 Model-based optimization of the recombinant protein production in *Pichia pastoris* based on dynamic flux balance analysis and elementary process functions 2815  
**Victor N. Emenike, Moritz Schulze, René Schenkendorf and Ulrike Krewer (Victor N. Emenike)**
- 09:10 Separation and recovery of intracellular beta-carotene using a process synthesis framework 2851  
**Alexander M. Sabol, Maria-Ona Bertran, Jonathan P. Raftery, John M. Woodley, Rafiqul Gani and M. Nazmul Karim (Alexander M. Sabol)**
- 09:30 Improving the Prediction of Phosphate Dynamics in Biotechnological Processes: A Case Study Based on Antibiotic Production Using *Streptomyces coelicolor* 2869  
**Patrick Bürger, Xavier Flores-Alsina, Harvey Arellano-Garcia and Krist V. Gernaey (Patrick Bürger)**

**Room B4**

**Chairpersons: Prof. Yasunori Kikuchi and Prof. Davide Manca**

**T6.- Concepts, Methods and Tools**

- 08:30 Source Code Generation for Parallelized Simulations of Large-Scale Nonlinear Equation Systems on a Supercomputer using MOSAIC, PETSc, and ADOL-C 2083  
**Henning Bonart, Sandra Fillinger, Erik Esche, Günter Wozny and Jens-Uwe Repke (Henning Bonart)**
- 08:50 Dynamic Optimization of Constrained Semi-Batch Processes Using Pontryagin's Minimum Principle and Parsimonious Parameterization 2041  
**Erdal Aydin, Dominique Bonvin and Kai Sundmacher (Erdal Aydin)**
- 09:10 Process Analysis on Multiple Solutions of Semi-algebraic Systems 2059  
**Fei Zhao, Xi Chen and Lingyu Zhu (Fei Zhao)**
- 09:30 When Robust Statistics Meets with Robust Optimization: Data-Driven Batch Process Scheduling in the Presence of Outliers 2263  
**Chao Ning and Fengqi You (Chao Ning)**



## 10:00 - 11:00 || WCCE Plenary

### Main Auditorium

10:00 *Process Research in the Chemical Industry*

**Peter Schuhmacher**

**President, Process Research & Chemical Engineering**

**BASF, Germany**

## 11:00 - 11:30 || Coffee Break

### Hall

## 11:30 - 13:10 || ESCAPE Lectures

### Room C2

Chairpersons: Prof. Natalia Menshutina and Dr. Jordi Bonet

### T1.- Modeling and Simulation

- 11:30 *Effect of Physical Properties on Accuracy Enhancement of Free Radical Polymerization Model in Tubular Reactors* 139  
**Arthit Vongachariya, Choosak Kiwjaroen, Kusuma Kulajanpeng, Siricharn Jirapongphan, Nattawat Tiensai and Wiwut Tanthapanichakoon (Arthit Vongachariya)**
- 11:50 *Modelling the physical properties of ionic liquid/metal salt mixtures with the soft-SAFT equation of state: application to carbon monoxide reactive separation* 217  
**Gabriel Zarca, Inmaculada Ortiz, Ane Urtiaga and Fèlix Llovell (Gabriel Zarca)**
- 12:10 *PU foams: Modelling of heat insulation properties and their degradation in time* 475  
**Pavel Ferkl, Andra Nistor, Martina Podivinska, Michal Vonka and Juraj Kosek (Pavel Ferkl)**
- 12:30 *Robust Flash Calculations through Nonsmooth Inside-Out Algorithms* 235  
**Harry A. J. Watson, Matias Vikse, Truls Gundersen and Paul I. Barton (Harry A. J. Watson)**
- 12:50 *Data Validation and Modelling of Thermodynamic Properties of Systems with Active Pharmaceutical Ingredients (APIs) in Complex Media for Skin Absorption Process* 247  
**Lukasz Ruszczynski, Alexandr Zubov, Gürkan Sin and Jens Abildskov (Lukasz Ruszczynski)**

### Room C5

Chairpersons: Prof. Il Moon and Prof. Peter Mizsey

### T2.- Synthesis and Design

- 11:30 *Optimal Shale Gas Flowback Water Desalination under Correlated Data Uncertainty* 943  
**Viviani C. Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, Alba Carrero-Parreño, Juan A. Reyes-Labarta and José A. Caballero (Jose A. Caballero)**
- 11:50 *Simulation-optimisation-based Design of Crude Oil Distillation Systems with Preflash Units* 823  
**Minerva Ledezma-Martínez, Megan Jobson and Robin Smith (Minerva Ledezma-Martínez)**
- 12:10 *Dynamic Modelling and Optimization of Acetylene Hydrogenation Reactor to Improve Overall Economics of Ethylene Plant* 847  
**Hattachai Aeowjaroenlap, Kritsada Chotiwiwiyakun, Nattawat Tiensai, Wiwut Tanthapanichakoon, Stepan Spatenka and Alejandro Cano (Hattachai Aeowjaroenlap)**
- 12:30 *Inherent Safety Evaluation for Process Flowsheets of Natural/Shale Gas Processes* 1243  
**Andrea P. Ortiz-Espinoza, Arturo Jiménez-Gutiérrez and Mahmoud M. El-Halwagi (Andrea P. Ortiz-Espinoza)**



- 12:50 Smart software system solution for model-based hazard identification of complex industrial processes 1225  
**Ján Janošovský, Matej Danko, Juraj Labovský and Ľudovít Jelemenský (Ján Janošovský)**

**Room C3**

**Chairpersons: Dr. Gonzalo Guillen Gosalbez and Dr. Ana Carvalho**

**T3.- Planning and Scheduling**

- 11:30 A decomposition framework for distribution of fluid products by a vendor-managed-inventory methodology 1387  
**Mariana Coccola, Carlos Alberto Méndez and Rodolfo Dondo (Carlos Alberto Méndez)**
- 11:50 Decision Automation for Oil and Gas Well Startup Scheduling Using MILP 1399  
**Jeffrey D. Kelly, Brenno C. Menezes and Ignacio E. Grossmann (Brenno C. Menezes)**
- 12:10 Optimal scheduling for power-intensive processes under time-sensitive electricity prices 1423  
**Natalia P. Basán, Ignacio E. Grossmann, Ajit Gopalakrishnan, Irene Lotero and Carlos Alberto Méndez (Natalia P. Basán)**
- 12:30 Efficient Precedence-Based Multistage Batch Scheduling Formulation with Nontrivial Tightening Constraints 1429  
**Pablo A. Marchetti and Jaime Cerdá (Pablo A. Marchetti)**
- 12:50 Synthesis of Supply Networks over Multiple Time Frames: A Case Study of Electricity Production from Biogas 1447  
**Jafaru Egieya, Lidija Čuček, Adeniyi Isafiade and Zdravko Kravanja (Jafaru Egieya)**

**Room C4**

**Chairpersons: Prof. Francisco Javier Recasens and Dr. Vincent Gerbaud**

**T5.- Integrated/Holistic approaches**

- 11:30 Systematic decision making models through Conceptual Constraints 1873  
**Canan Dombayci and Antonio Espuña (Canan Dombayci)**
- 11:50 Integrated Design, Planning, and Scheduling of Renewables-based Fuels and Power Production Networks 1879  
**Qi Zhang, Mariano Martín and Ignacio E. Grossmann (Qi Zhang)**
- 12:10 Shared resource allocation in the process industries via price-based coordination for systems with discrete decisions 1897  
**Lukas Samuel Maxeiner, Simon Wenzel and Sebastian Engell (Lukas Samuel Maxeiner)**
- 12:30 Incorporating detailed metabolic models into superstructure optimization of biorefineries 2143  
**Amir Akbari and Paul I. Barton (Amir Akbari)**
- 12:50 Model-based multi-parametric programming strategies towards the integration of design, control and operational optimization 1867  
**Nikolaos A. Diangelakis and Efstratios N. Pistikopoulos (Nikolaos A. Diangelakis)**

**Room D2**

**Chairpersons: Prof. Alberto Bandoni and Prof. Krist Gernaey**

**T7.- CAPE applications addressing Global Grand Challenges**

- 11:30 Identifying Gene Regulatory Networks 2749  
**Aristotelis Kittas, Lingjian Yang, Lazaros G. Papageorgiou, Gill May, Tariq Enver and David Bogle (David Bogle)**
- 11:50 A Population Balance Model for Stem Cell Differentiation Bioprocesses 2761  
**Romuald György, Michail E. Klontzas, Margaritis Kostoglou, Nicki Panoskaltzis, Athanasios Mantalaris and Michael C. Georgiadis (Romuald György)**



- 12:10 *A Model-Based Support for Diagnosing von Willebrand Disease* 2779  
**Christopher Castaldello, Alessio Gubert, Federico Galvanin, Alessandra Casonato, Roberto Padrini, Massimiliano Barolo and Fabrizio Bezzo (Fabrizio Bezzo)**
- 12:30 *Risk Evaluation Models for the Design of Parenterals Manufacturing Processes* 2791  
**Haruku Shirahata, Masahiko Hirao and Hirokazu Sugiyama (Haruku Shirahata)**
- 12:50 *Dynamic Optimization of Continuous Manufacturing of Pharmaceuticals* 2803  
**Michael Shoham Patrascu and Paul I. Barton (Michael Shoham Patrascu)**

### **13:10 - 14:30 || Lunch**

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Catering Area

### **14:30 - 15:30 || WCCE Plenary**

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Main Auditorium

- 14:30 **James (Jim) R. Fitterling**  
*Chief Operating Officer for the Materials Science Division*  
*DowDuPont, USA*

### **15:30 - 16:00 || Coffee Break**

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Hall

### **16:00 - 18:00 || Closing / Awards**

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Main Auditorium

