ESCAPE-27 Barcelona October 1st - 5th 2017

European Symposium on Computer-Aided Process Engineering

WCCE10 ECCE11 ECAB4

European Symposium on Computer-Aided Process Engineering

Fira de Barcelona, Hall 8, Barcelona, Spain

01 – 05 October, 2017

Scientific Program

(Link 1: map)

(updated: September 30th , 2017)

(Link 2: view)

GENERAL VIEW

01/10/2017	02/10/2017	03/10/2017	04/10/2017	05/10/2017
	Registration (08:00 -20:00)	Registration	Registration	Registration
	Opening / Awards (09:00-10:00)	ESCAPE Lectures 4 lectures (x 5) (08:30-09:50)	ESCAPE Lectures 4 lectures (x 5) (08:30-09:50)	ESCAPE Lectures 4 lectures (x 6) (08:30-09:50)
	ESCAPE / WCCE Plenary	WCCE Plenary	WCCE Plenary	WCCE Plenary
	Coffee Break / Posters (11:00 - 11:45)	Coffee Break / Posters (11:00 - 11:45)	Coffee Break / Posters (11:00 - 11:45)	Coffee Break
	ESCAPE Keynotes 2 keynotes (x3)	ESCAPE Keynotes 3 keynotes (x3) (11:50 - 13:20)	ESCAPE Lectures 4 lectures (x5) (11:50 - 13:10)	ESCAPE Lectures 5 lectures (x5) (11:30 - 13:10)
	Lunch (13:00-14:30)	Lunch (13:20-14:30)	Lunch (13:10-14:30)	Lunch (13:10-14:30)
	ESCAPE / WCCE Plenary	ESCAPE / WCCE Plenary	WCCE Plenary	WCCE Plenary
	Coffee Break / Posters (15:30 - 16:25)	Coffee Break / Posters (15:30 - 16:25)	Coffee Break / Posters (15:30 - 16:25)	Coffee Break
	ESCAPE Lectures (16:30-19:00)	ESCAPE Lectures (16:30-19:00)	ESCAPE Lectures (16:30-18:10)	Closing / Awards (16:00-18:00)
Welcome / Party (17:00-19:00)	Cheese&Wine reception			

PhD Networking Party	Gala Dinner

01, Sunday

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

Room: E2 (2nd floor)

15:00 - 19:00 || Registration

Registration Desk

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

Main Hall of the Congress Venue

02, Monday

08:00 - 20:00 || Registration

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
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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)

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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)

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Hasan Jafari, Amir Sheikhi and Rahmat Sotudeh-Gharebagh (Rahmat Sotudeh-Gharebaagh)

P1.08 *Modelling of an adiabatic trickle-bed reactor with phase change* 115
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Catarina G. Braz, Henrique A. Matos, A. Mendes, Jorge F. Rocha and Ricardo P. Alvim (A. Catarina Braz)

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Botond Szilagyi, Akos Borsos, Elena Simone and Zoltan K. Nagy (Botond Szilagyi)

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P1.16 *Software Tool for Computing and Visualization of Enhanced Residue Curve Maps* 199
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P1.17 *A Systematic Identification Method for Thermodynamic Property Modelling* 205
Olivia A. Perederic, Larissa P. Cunico, Bent Sarup, John M. Woodley and Rafiqul Gani (Olivia A. Perederic)

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P1.19 *Characterisation of axial dispersion in a Meso-scale Oscillatory Baffled Crystalliser using a Numerical Approach* 223
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Nataliya Shcherbakova, Ivonne Rodriguez–Donis, Jens Abildskov and Vincent Gerbaud (Nataliya Shcherbakova)

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Poster Hall (P2)

T2.- Synthesis and Design

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Žan Zore, Klavdija Zirngast, Zorka Novak Pintarič and Zdravko Kravanja (Žan Zore)

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P2.04 *Infeasible Path Global Flowsheet Optimization Using McCormick Relaxations* 631
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P2.05 *A MOO approach towards sustainable process design: integrating the three pillars of sustainability* 637
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P2.10 *A Framework for an Optimized Sustainable Product and Process Design: Acetone-Butanol-Ethanol Separation and Purification* 697
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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)

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P2.17 *Heat Exchanger Network Retrofit with Fouling Effects* 775
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P2.18 *Multi-objective optimization of utility systems and heat exchanger networks: method and application to the solar-assisted hydrothermal gasification case* 781
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P2.19 *Modelling, Simulation and Economical Evaluation of Dry Food Manufacture at Different Production Scales.* 787
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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
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T3.- Planning and Scheduling

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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
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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
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P3.07 *Optimal Production Planning and Crude Oil Blending in a Conventional Oilfield* 1309
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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 Pessemier, 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)

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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
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P3.19 *CLSC design with simultaneous consideration of product design for manufacturing and remanufacturing* 1453
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Poster Hall (P6)

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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 Lignocellulsic 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, Moisès 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
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Poster Hall (P7)

T7.- CAPE applications addressing Global Grand Challenges

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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 Lützow, Dinah Elena Majewski, Matthias Lampe, Maike 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_2 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 (Deepa Elizabeth Eapen)

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 (CAPE-WP Long Term Acheivement Award)
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 (2nd 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_2–rich Natural Gas using Fischer-Tropsch Synthesis Coupled to Tri-reforming Process* 2659
José E. A. Graciano, André D. Carreirra, 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_2 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_2 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 - 20:00 || Registration

Registration Desk .

08:00 - 18:00 || Posters

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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 Tyrtyshnikov, 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 (Andrea König)

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, Moisès 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
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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 Baltsas 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™ 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
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Yeong-Gak Yoon, Dae-Sung Song and Chul-Jin Lee (Yeong-Gak Yoon)
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Xinyan Liu, Xiaodong Liang, Rafiqul Gani, Xiangping Zhang and Suojiang Zhang (Xinyan Liu)

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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-Rodriguez (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)

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T5.- Integrated/Holistic approaches

P5.01 *Integrated process and solvent design using COSMO-RS for the production of CO from CO_2 and H_2* 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, Raphaele 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
Ségolène Belletante, Ludovic Montastruc, Stéphane Negny, Raphaele 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_2 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 Espuña (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 Harjunkoski (Iiro Harjunkoski)

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 Heinzel, 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
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P6.29 *Knowledge-Driven Multi-Label Classification of Process Scheduling Problems* 2353
Elisabet Capón-García, Edrisi Muñoz, José Miguel Laínez-Aguirre and Konrad Hungerbühler (Elisabet Capon-Garcia)
P6.30 *Constraint Identification and Integration Procedures in Multi-Level Hierarchical Systems* 2359
Canan Dombayci, Elisabet Capón-García, Edrisi Muñoz and Antonio Espuña (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_2 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_2 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_2 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_2 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_2 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_2 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: Técnicas Reunidas experience*
Miguel Pardinas
Deputy CEO
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_2 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-Gosálvez)

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

12:20 *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 (2nd 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 Hasseine and Hans-Jörg Bart (Samer Alzyod)

16:50 *Population balance modelling of pulsed packed bed extraction columns using PPBLab software* 67
Menwer Attarakih, Samer Alzyod and Armin Fricke (Menwer Attarakih)

17:10 *Particle Size Effects on Collision and Agglomeration in Turbulent Channel Flows* 79
Tosanbami Ogholaja, Derrick O. Njobuenwu and Michael Fairweather (Tosanbami Ogholaja)

17:30 *Modelling of Droplet Absorption and Evaporation during Pharmaceutical Tablet Coating* 85
Charalampos Christodoulou, Luca Mazzei, Salvador García-Muñoz and Eva Sorensen (Charalampos Christodoulou)

17:50 *Random porous network generation and 1D mass transfer simulation for gamma-alumina supports* 91
Sónia Ferreira, Jan J. Verstraete, Elsa Jolimaitre, Damien Leinekugel-Le-Cocq and Christian Jallut (Sónia Ferreira)

18:10 *Large Eddy Simulation of Microbubble Transport in Vertical Channel Flows* 73
Kenneth S. Asiagbe, Michael Fairweather, Derrick O. Njobuenwu and Marco Colombo (Kenneth S. Asiagbe)

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* 1033
Juan Javaloyes-Anton, Sergio Ferrer-Nadal, Ignacio Vic and José A. Caballero (Juan Javaloyes-Anton)

16:50 *Hedging Against Uncertain Feedstock Compositions in Shale Gas Processing System Designs with Intensified Equipment Capacities* 1051
Jian Gong and Fengqi You (Jian Gong)

17:10 *Novel Reactive Distillation Processes to produce Diphenyl Carbonate: Multi-Objective Optimization involving Cost and Controllability Criteria* 1069
Gabriel Contreras-Zarazúa, José Antonio Vazquez-Castillo, Cesar Ramirez-Marquez, Juan Gabriel Segovia-Hernández and Jesus Rafael Alcantara-Avila (Juan Gabriel Segovia-Hernandez)

17:30 *Design and Control of Processes for 2-Ethylhexyl Acrylate Production* 1087
Mihai Daniel Moraru and Costin Sorin Bildea (Mihai Daniel Moraru)

17:50 *Innovative design and simulation of a castor oil biorefinery* 1111
Alexandre Corneliu Dimian, Petrica Iancu, Valentin Plesu, Alexandra-Elena Bonet-Ruiz and Jordi Bonet (Petrica Iancu)

18:10 *Model-Based Analysis and Integration of Synthetic Methane Production and Methane Oxidative Coupling* 1147
Estelle le Sache, Yang Peng, Harvey Arellano-Garcia and Tomas Ramirez Reina (Tomas Ramirez Reina)

18:30 *A simplified kinetic and mass transfer modelling of the thermal hydrolysis of vegetable oils* 1177
Hector Forero-Hernandez, Mark Jones, Bent Sarup, Jens Abildskov, Anker D. Jensen and Gürkan Sin (Hector Forero-Hernandez)

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* 1921
Sergio Medina-González, Fengqi You and Antonio Espuña (Sergio Medina-González)

16:50 *Systematic decision making methodology for chemical product design in integrated biorefineries* 1771
Yen Yi Lai, Kelvin Chu How Yik, Han Peng Hau, Chai Peng Chow and Lik Yin Ng (Lik Yin Ng)

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, Raphaele 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 Bourdiec (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 Espuña and Luis Puigjaner (Elisabet Capón-Garcia)

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 Geraldes (Henrique A. Matos)

20:30 PhD Networking Party

Poble Espanyol (link)

04, Wednesday

08:00 - 20:00 || Registration

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_2 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 (Maria 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. Bähner, Paloma A. Santacoloma, Jens Abildskov and Jakob K. Huusom (Franz D. Bähner)

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* 1483
Ines V. Stelzer, Julian Kager and Christoph Herwig (Ines V. Stelzer)

P4.05 *A model for subsea oil-water gravity separator to estimate unmeasured disturbances* 1489
Tamal Das, Christoph Josef Backi and Johannes Jäschke (Tamal Das)

P4.06 *Profile-driven Features for Offline Quality Prediction in Batch Processes* 1501
Ricardo Rendall, Bo Lu, Ivan Castillo, Swee-Teng Chin, Leo H. Chiang and Marco S. Reis (Tiago J. Rato)

P4.07 *Optimal Sensor Network Design to Monitor the Energy Performances of a Process Plant* 1507
Hala Rameh, Cong-Toan Tran, Assaad Zoughaib, Marie-Ann Evans and Jean-Paul Gourlia (Hala Rameh)

P4.08 *A robust methodology for the sensor fault detection and classification of systematic observation errors* 1525
Claudia E. Llanos, Mabel C. Sánchez and Ricardo A. Maronna (Claudia E. Llanos)

P4.09 *Smith predictor for slug control with large valve stroke time* 1531
Henry Tandoh, Yi Cao and Adeola Awoyomi (Henry Tandoh)

P4.10 *An efficient and rigorous thermodynamic library and optimal-control of a cryogenic air separation unit* 1543
Jozsef Gaspar, Tobias K. S. Ritschel and John Bagterp Jørgensen (Jozsef Gaspar)

P4.11 *Process control of a heat pump assisted extractive DWC for bioethanol dehydration* 1549
Iulian Patraşcu and Costin Sorin Bîldea (Costin Sorin Bildea)

P4.12 *Dynamic simulation of thermal energy storage integrated with small-scale solar power plant and organic Rankine cycle* 1561
Sittiporn Vongsilodkul and Soorathep Kheawhom (Soorathep Kheawhom)

P4.13 *Economic Predictive Control of a Pasteurization Plant using a Linear Parameter Varying Model* 1573
Fatemeh Karimi Pour, Vicenç Puig and Carlos Ocampo-Martinez (Fatemeh Karimi Pour)

P4.14 *Advanced Robust MPC Design of a Heat Exchanger: Modeling and Experiments* 1585
Juraj Oravec, Monika Bakošová, Daniela Pakšiová, Natália Mikušová and Kinga Batárová (Juraj Oravec)

P4.15 *A multi-parametric bi-level optimization strategy for hierarchical model predictive control* 1591
Styliani Avraamidou and Efstratios N. Pistikopoulos (Styliani Avraamidou)

P4.16 *A novel back-up control structure to manage non-routine steam upsets in industrial methanol distillation columns* 1597
Isuru A. Udugama, Coromina Zander, Seyed Soheil Mansouri, Robert Kirkpatrick, Wei Yu and Brent R. Young (Wei Yu)

P4.17 *Identification and Model Predictive Control Design of a Polymer Extrusion Process* 1609
Ioannis Meintanis, George Halikias, Roberto Giovenco, Andreas Yiotis and Kostas Chrysagis (Ioannis Meintanis)

P4.18 *Tuning of PI controllers by Differential Evolution with Tabu List method* 1633
Cesar Ramirez-Marquez, Erick Yair Miranda-Galindo, Juan Gabriel Segovia-Hernández and Salvador Hernández (Juan Gabriel Segovia-Hernandez)

P4.19 *Set point tracking of a biogas plant coupled to a methanation reactor* 1645
Andreas Himmel, Sebastian Sager and Kai Sundmacher (Andreas Himmel)

P4.21 *Sliding Dynamic Data Window: Improving Properties of the Incremental Learning Methods* 1663
Mohammad Hamed Ardakani, Gerard Escudero, Moisès Graells and Antonio Espuña (Mohammad Hamed Ardakani)

P4.22 *Process Fault Isolation via Bayesian Lasso-based Reconstruction Analysis* 1669
Zhengbing Yan and Yuan Yao (Yuan Yao)

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 remifentanil 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* 2827
Tannaz Tajsoleiman, Daria Semenova, Ana C. Fernandes, Jakob Kjøbsted Huusom, Krist V. Gernaey and Ulrich Krühne (Tannaz Tajsoleiman)

P7.57 *Kinetic Modelling and Scaled-up Experimental Studies of Microalgal Fuels and Chemicals Production* 2833
Mesut Bekirogullari, Jon K. Pittman and Constantinos Theodoropoulos (Constantinos Theodoropoulos)

P7.58 *Modelling of the imperfect mixing in a hybrid exothermic chemical reactor with simulated heat of reaction* 2845
Piotr Skupin, Mieczyslaw Metzger, Piotr Laszczyk and Malgorzata Niedzwiedz (Piotr Skupin)

P7.59 *Metabolic Network design of Synechocystis sp. PCC 6803 to obtain bioethanol under autotrophic conditions* 2857
Romina Lasry Testa, Claudio Delpino, Vanina Estrada and Maria Soledad Diaz (Maria Soledad Diaz)

P7.60 *Transesterification of Castor Oil Catalyzed by Liquid Enzymes: Optimization of Reaction Conditions* 2863
Thalles Allan Andrade, Massimiliano Errico and Knud Villy Christensen (Thalles Allan Andrade)

P7.61 *Experimental Work Towards the Improvement of a Kinetic Model for Acetone-Butanol-Ethanol Pathway* 2875
Asal Rahimsalehi, Claudio Avignone-Rossa and Harvey Arellano-Garcia (Harvey Arellano-Garcia)

P7.62 *Modeling Biodiesel Production and Purification – Towards a Predictive Tool* 2881
Lourdes F. Vega, Felix Llovell, J. Torné, S. V. D. Freitas, Mariana B. Oliveira and Joao A. P. Coutinho (Lourdes F. Vega)

P7.63 *Attainable Region for Biobutanol Production* 2893
Cansu Birgen, Heinz A. Preisig, Alexander Wentzel, Sidsel Markussen and Bernd Wittgens (Cansu Birgen)

P7.64 *Heat integration for the production process of 2G bioethanol from wheat straw* 2917
Moises Gonzalez-Contreras, Arturo Sanchez and Teresa Lopez-Arenas (Moises Gonzalez-Contreras)

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_2 Methanation Reactor* 127
Karsten Hans Georg Rätze, Jens Bremer, Lorenz T. Biegler and Kai Sundmacher (Karsten Hans Georg Rätze)

08:50 *Fouling Modelling in Crude Oil Preheat Systems* 409
José Loyola-Fuentes, Robin Smith and Megan Jobson (Jose Loyola-Fuentes)

09:10 *Development and Optimization of a Single Column Analog Model for a Multi-Column Counter-Current Solvent Gradient Purification Process* 187
Anton Sellberg, Niklas Andersson, Anders Holmqvist and Bernt Nilsson (Anton Sellberg)

09:30 *Crystallization of Calcium Carbonate and Magnesium Hydroxide in the Heat Exchangers of Once-through Multistage Flash Process Desalination* 349
Salih Alsadaie and Iqbal M. Mujtaba (Iqbal M. Mujtaba)

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. Giorgos Kopanos**

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 *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)

09:30 *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)

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 Elsido, Alberto Mian, François Maréchal and Emanuele Martelli (Cristina Elsido)

09:10 *Optimal design and operation of A-frame systems for solar power plants* *2449*
José Antonio Luceño and Mariano Martín (Mariano Martin)

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, Mahdieh Askarian, Gerard Escudero, Moisès Graells and Antonio Espuña (Mahdieh 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 Nougués (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 Smulation

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 Szijjarto 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. Hirokazu Sugiyama Prof. Diego Cafaro**

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. Promentilla, Kathleen B. Aviso and Raymond R. Tan (Michael Angelo B. Promentilla)

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

Hall

20:30 … || Gala Dinner

Maritime Museum - Drassanes Reials (link)

05, Thursday

08:00 - 18:30 || Registration

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 Bourdiec (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 Dr. Tibor Nagy**

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 Chotiwiriyakun, 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 Panoskaltsis, 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

Catering Area

14:30 - 15:30 || WCCE Plenary

Main Auditorium

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

15:30 - 16:00 || Coffee Break

Hall

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

Main Auditorium