

PSE-2015/ESCAPE-25

31 May – 4 June 2015

Bella Center, Copenhagen, Denmark

Sunday May 31st, 2015

10:30-17:00 CAPE-WP

Business meeting (Bell Center, room 17)

12:00 – 13:00 Lunch for CAPE-WP

14:00-14:30 Registration opens (Bella Center)

18:00- Reception (Bella Center)

Monday June 1st, 2015

08:30-08:50 Opening session (A11+A12)

08:50-09:50 Plenary 1 (A11+A12):

Chair: Efstratios N. Pistikopoulos

08:50 Recent Advances in Mathematical Programming Techniques for the Optimization of Process Systems under Uncertainty 1132
Prof Ignacio Grossmann, Carnegie Mellon University, Pittsburgh, USA

09:50-10:30 Break (Hall A)

10:30-12:10 Parallel Session: Enterprise-wide Management (Oral A1.1, T-8.1, A11)

Chair: Antonio Espuña, Christos T. Maravelias

10:30 Product and Process Network Modelling and Pathway Optimization with Life Cycle Analysis: The Case of Biofuels 1000
Daniel Garcia, Fengqi You

10:50 Interplant carbon integration towards phased footprint reduction targets 944
Dhabia M. Al-Mohannadi, Patrick Linke, Sumit K. Bishnu, Sabla Y. Almouri

11:10 Decision Support by Multicriteria Optimization in Process Development: An Integrated Approach for Robust Planning and Design of Plant Experiments 97
Michael Bortz, Volker Maag, Jan Schwientek, Regina Benfer, Roger Böttcher, Jakob Burger, Erik von Harbou, Norbert Asprion, Karl-Heinz Küfer, Hans Hasse

11:30 Agent-based model of the German Biodiesel Supply Chain 84
Jorge A. Moncada, Martin Junginger, Zofia Lukszo, André Faaij, Margot Weijnen

11:50 A study on sustainable development of China's phosphorus resources industry based on system dynamics 428
Shujie Ma, Shanying Hu, Dingjiang Chen, Yuzhong Feng

10:30-12:10 Parallel Session: PSE education (Oral A1.2, T-0, A12)

Chair: Ian T. Cameron, Ka M. Ng

10:30 Incorporating Process Synthesis in the Processing Systems Design Course 117
Jeffrey J. Siirola, Carnegie Mellon University & Purdue University, USA (Keynote)

11:10 Process Simulators: What Students Forget When Using Them, Their Limitations, and When Not to Use Them 392
Joseph A. Shaeiwitz, Richard Turton

11:30 Learning to solve mass balance problems through a web-based simulation environment 573
Alexandros Koulouris, Dimitrios Vardalis

11:50 A Framework to Structure Operational Documents for Chemical Processes 919
Hiroshi Osaka, Yuji Naka, Tetsuo Fuchino

10:30-12:10 Parallel Session: Industrial Control Applications (Oral A1.3, T-5.2, 19)

Chair: Sebastian Engell, I-Lung Chien

10:30 Semi-global stabilization of polymerization processes using extended washout filter-aided controller 1147

	<i>Nan Zhang, Warren D. Seider, Chen Bingzhen</i>	
10:50	Systematic Control Structure Evaluation of Two-Stage-Riser Fluidized Catalytic Pyrolysis Processes <i>Zhihong Yuan, Ping Wang, Mario R. Eden</i>	791
11:10	Robust Model Predictive Control Strategy for LTV and LPV Systems of the Internal Reforming Solid Oxide Fuel cell <i>Narissara Chatrattanawet, Soorathep Kheawhom, Amornchai Arpornwichanop</i>	839
11:30	Energy Optimization in Pasteurization Processes <i>Patrick Hammer, Martin Mayer, Stefan Jakubek</i>	470
11:50	Dynamic Simulation and Analysis of Slug Flow Impact on Offshore Natural Gas Processing: TEG Dehydration, Joule-Thomson Expansion and Membrane Separation <i>Lara de O. Arinelli, Ofélia Q. F. Araújo, José L. de Medeiros</i>	1068
10:30-12:10	Parallel Session: Biological Systems Engineering (Oral A1.4, T-9.2, 18) <i>Chair: John M. Woodley, Jean-Marc Le Lann</i>	
10:30	Manufacturability Indices for High-Concentration Monoclonal Antibody Formulations <i>Yang Yang, Ajoy Velayudhan, Nina F. Thornhill, Suzanne S. Farid</i>	604
10:50	Enzymatic Reactive Distillation for the Transesterification of Ethyl Butyrate: Model Validation and Process Analysis <i>Matthias Wierschem, Rene Heils, Stefan Schlimper, Irina Smirnova, Andrzej Górak, Philip Lutze</i>	480
11:10	Development of a Macroscopic Model for the Production of Bioethanol with High Yield and Productivity via the Fermentation of <i>Phalaris aquatica</i> L. Hydrolysate <i>Anna Karapatsia, Giannis Penloglou, Christos Chatzidoukas, Costas Kiparissides</i>	475
11:30	Robust process design for the bioproduction of beta-carotene in green microalgae <i>Robert J. Flassig, Melanie Fachel, Liisa Rihko-Struckmann, Kai Sundmacher</i>	325
11:50	Proposal of a New Pathway for Microalgal Oil Production and its Comparison with Conventional Method <i>Sofia Chaudry, Parisa A. Bahri, Navid R. Moheimani</i>	520
10:30-12:10	Parallel Session: Power Systems Planning (Oral A1.5, T-9.5.4, 20) <i>Chair: Michael C. Georgiadis, Iftekhar A. Karimi</i>	
10:30	Integrated Solar Thermal Hydrogen and Power Coproduction Process for Continuous Power Supply and Production of Chemicals <i>Emre Gençer, Mohit Tawarmalani, Rakesh Agrawal</i>	418
10:50	Structural similarities and differences between smart grids and process industry supply chains: India case study <i>Nikita Patel, Rishabh Abhinav, Babji Srinivasan, Rajagopalan Srinivasan</i>	849
11:10	Bringing non-energy systems into bioenergy value chain optimization framework <i>Miao Guo, Nilay Shah</i>	683
11:30	Optimal integration of the year-round operation for methane production from CO ₂ and water using wind, solar and biomass <i>Mariano Martín, William Davis</i>	205
11:50	A computer-aided scenario analysis of future energy demand/supply systems: A case study in Japan	415

Yasunori Kikuchi, Yuichiro Kanematsu, Yoshifumi Takayama, Michihisa Koyama, Yutaka Genchi, Masahiko Hirao

10:30-11:30 Oral Highlights I (17)

Chair: Loïc d'Anterroches

Posters 385, 62, 72, 296, 304, 322, 660, 1110, 1144, 469, 790, 1114

12:10-13:00 Lunch (Hall A)

13:00-14:40 Parallel Session: Numerical Issues (Oral B1.1, T-1.4, A11)

Chair: Sten B. Jørgensen, Fabrizio Bezzo

13:00 Automatic reconstruction and generation of structured hexahedral mesh for non-planar bifurcations in vascular network 986
Mahsa Ghaffari, Chih-Yang Hsu, Andreas A. Linninger

13:20 Reformulating The Minimum Eigenvalue Maximization In Optimal Experiment Design Of Nonlinear Dynamic Biosystems 627
Dries Telen, Nick Van Riet, Filip Logist, Jan Van Impe

13:40 Differential-Algebraic Approach to Solve Steady-State Two-Phase Flow Drift-Flux Model with Phase Change 412
Rodrigo G. D. Teixeira, Argimiro R. Secchi, Evaristo C. Biscaia Jr.

14:00 Parallel Computation Method for Solving Large Scale Equation-oriented Models 238
Yannan Ma, Jinzu Weng, Zhijiang Shao, Xi Chen, Lingyu Zhu, Yuhong Zhao

14:20 Uncertainty in clinical data and stochastic model for in-vitro fertilization 10
Kirti M. Yenkie, Urmila M. Diwekar

13:00-14:40 Parallel Session: Product Synthesis-Design (Oral B1.2, T-4.4, A12)

Chair: Kyle V. Camarda, Mariano Martín

13:00 Discovery of New Zeolites for H₂S Removal through Multi-scale Systems Engineering 86
Tingting Liu, Eric L. First, M. M. Faruque Hasan, Christodoulos A. Floudas

13:20 Integrated Product and Process Design for the Optimization of Mayonnaise Creaminess 318
Arend Dubbelboer, Jo Janssen, Ardjan Krijgsman, Edwin Zondervan, Jan Meuldijk

13:40 Integrated Design of Working Fluid, Process and Turbine of Organic Rankine Cycles using PC-SAFT 629
Matthias Lampe, Joachim Gross, Piero Colonna, André Bardow

14:00 A systematic visual approach to ionic liquid design for carbon dioxide capture 414
Fah K. Chong, Nishanth G. Chemmangattualappil, Dominic C. Y. Foo, Mert Atilhan, Fadwa T. Eljack

14:20 Designing Reactants and Products with Properties Dependent on Both Structures 1084
Vikrant A. Dev, Nishanth G. Chemmangattualappil, Mario R. Eden

13:00-14:40 Parallel Session: Control of Column Processes (Oral B1.3, T-5.4, 19)

Chair: Sigurd Skogestad, Teresa Lopez-Arenas

13:00 A control strategy for periodic systems - application to the twin-column MCSGP 64
Maria M. Papathanasiou, Fabian Steinebach, Guido Stroehlein, Thomas Müller-Späth, Ioana Nascu, Richard Oberdieck, Massimo Morbidelli, Athanasios Mantalaris, Efstratios N. Pistikopoulos

13:20	Comparing Temperature Difference Control Schemes for Dividing-Wall Distillation Columns <i>Yang Yuan, Haisheng Chen, Jieping Yu, Kejin Huang</i>	25
13:40	Raman-based Advanced Control of an Absorption Desorption System <i>Erik Esche, David Müller, Michael Maiwald, Günter Wozny</i>	100
14:00	High purity, high recovery, multi-component methanol distillation control <i>Isuru A. Udugama, Tajammal Munir, Robert Kirkpatrick, Brent R. Young, Wei Yu</i>	410
14:20	Performance Evaluation of Bayesian State Estimators for Nonlinear DAE Systems Using a Moderately High Dimensional Reactive Distillation Column Model <i>Jalesh L. Purohit, Sachin C. Patwardhan, Sanjay M. Mahajani</i>	981
13:00-14:40	Parallel Session: Plant Operations (Oral B1.4, T-7.1, 18) <i>Chair: Metin Turkay, Iiro Harjunkoski</i>	
13:00	Optimal Management of Shuttle Robots in a Laboratory Automation System of a Cement Plant <i>Christian Schoppmeyer, Christian Sonntag, Siddharth Gajjala, Sebastian Engell</i>	280
13:20	Simultaneous optimisation of economic and environmental objectives with dynamic price signals and operational constraints <i>Tristan Lambert, Andrew F. A. Hoadley, Barry Hooper</i>	342
13:40	Integrated cyclic scheduling and operation optimization for cracking furnaces group considering feed changeover <i>Yangkun Jin, Jinlong Li, Wenli Du, Feng Qian</i>	714
14:00	A MILP transshipment model to integrate and re-engineer distillation columns into overall processes <i>Konstantinos A. Pyrgakis, Kipouros P. Ioannis, Antonis C. Kokossis</i>	1018
14:20	Optimization of petrochemical process planning using naphtha price forecast and process modeling <i>Kwon Hweeung, Lyu Byeonggil, Tak Kyungjae, Lee Jinsuk, Moon Il, Sunghyun Cho</i>	455
13:00-14:40	Parallel Session: Biorefineries and Fuels (Oral B1.5, T-9.5.1, 20) <i>Chair: Fengqi You, Flavio Manenti</i>	
13:00	Synthesis of Optimal Processing Pathway for Microalgae-based Biorefinery under Uncertainty <i>Muhammad Rizwan, Jay H. Lee, Rafiqul Gani</i>	516
13:20	Biorefinery process optimization and risk estimation at industrial level <i>Javier Pinedo, Carla Valeria García Prieto, Agustín Alejo D'alexandro, María Soledad Díaz, Stella Maris Tonelli, Raquel Ibáñez, Ángel Irabien</i>	689
13:40	Integrated Computational and Experimental Studies of Microalgal Production of Fuels and Chemicals <i>Mesut Bekirogullari, Jon Pittman, Constantinos Theodoropoulos</i>	850
14:00	Process Integration and Assessment of Biogas System <i>Bin Wu, Yajing Xu, Xiangping Zhang</i>	872
14:20	Optimum Facility Location and Plant Scheduling for Biofuel Production <i>Chen Li, Selen Cremaschi</i>	978
14:40-16:00	Elsevier Poster Session 1 (Hall A)	

16:00-17:30	Parallel Keynote Session: Pharma I (Key 1.1, A-2, A11) <i>Chair: Marianthi Ierapetritou</i>	
16:00	Modeling in API downstream process development <i>Roel Hoefnagels, Janssen, Belgium</i>	1138
16:30	Challenges and opportunities for process system modelling in the development of new medicines <i>Gavin K. Reynolds, AstraZeneca, UK</i>	1133
17:00	The role of Process Systems Engineers on designing sustainable products and processes <i>Concepción "Conchita" Jiménez-González, GlaxoSmithKline</i>	257
16:00-17:30	Parallel Keynote Session: Planning & Scheduling I (Key 1.2, A-1, A12) <i>Chair: Ignacio E. Grossmann</i>	
16:00	Industrial perspectives on deployment of scheduling solutions <i>Iiro Harjunkoski, ABB, Germany</i>	244
16:30	Processing Pathway/ Supply Chain Optimization Problems for Emerging Energy Technologies: Issues and Some Promising Directions <i>Jay H. Lee, KAIST, Korea</i>	32
17:00	Supply Chain Simulation: Creating Competitive Advantage for DSM <i>Dorus van der Linden, DSM, Holland</i>	28
16:00-17:30	Parallel Keynote Session: Industrial Problems (Key 1.3, A-6, 20) <i>Chair: Patrick M. Piccione</i>	
16:00	Modeling in Process Industry: Needs, Applications and Challenges <i>Konrad Triebeneck, Bayer Technology Services, Germany</i>	151
16:30	New Perspective of Simulation & Modeling to Accelerate Development of Petrochemical Products <i>Khavinet Louvranij, SCG Chemicals, Thailand</i>	1155
17:00	Advances and Challenges in Modelling of Processing of Lipids <i>Bent Sarup, Alfa Laval, Denmark</i>	1048
19:00-	Copenhagen Town Hall reception	

Tuesday June 2nd, 2015

08:30-10:30 Parallel Session: CFD/PBM (Oral A2.1, T-1.1, A11)

Chair: Ulrich Krühne, Davide Manca

- 08:30 Population balance model for enzymatic depolymerization of branched starch 139
Christoph Kirse, Heiko Briesen
- 08:50 OPOSSIM: A Population Balance-SIMULINK Module for Modelling Coupled 298
Hydrodynamics and Mass Transfer in Liquid Extraction Equipment
Menwer Attarakih, Samer Al-Zyod, Mark Hlawitschke, Hans-Jörg Bart
- 09:10 CFD-DEM simulation of a fluidized bed crystallization reactor 316
Kristin Kerst, Luis M. de Souza, Antje Bartz, Andreas Seidel-Morgenstern, Gábor Janiga
- 09:30 Application of the Lagrangian CFD Approach to Modelling of Crystallization in Stirred 976
Batch Reactors Using the Smoothed Particle Hydrodynamics Method
Dragan D. Nikolic, Brian P. de Souza, Patrick J. Frawley
- 09:50 A Meshfree Maximum Entropy Method for the Solution of the Population Balance 110
Equation
Menwer Attarakih, Abdelmalek Hasseine, Hans-Jörg Bart
- 10:10 Microalgae Growth Determination Using Breakage Equation Model 532
Ergys Pahija, Yu Zhang, Yi Zhu, Chi W. Hui

08:30-10:30 Parallel Session: Process Synthesis of Biorefineries (Oral A2.2, T-4.1, A12)

Chair: Fernando L. P. Pessoa, Selen Cremaschi

- 08:30 A Novel Approach for the Identification of Economic Opportunities within the 391
Framework of a Biorefinery
Ana I. Torres, Iwona Cybulska, Chuanji Fang, Mette H. Thomsen, Jens E. Schmidt, George Stephanopoulos
- 08:50 Using Product Driven Process Synthesis in the Bio-refinery 566
Alexandra Kiskini, Edwin Zondervan, Peter Wierenga, Edwin Poiesz, Harry Gruppen
- 09:10 Value-added Chemicals from Microalgae: A Sustainable Process Design Using Life Cycle 1008
Optimization
Jian Gong, Fengqi You
- 09:30 Natural Gas to Liquid Transportation Fuels and Olefins (GTL+C2_C4) 508
Onur Onel, Alexander M. Niziolek, Christodoulos A. Floudas
- 09:50 Optimization and Analysis of Chemical Synthesis Routes for the Production of Biofuels 272
Douglas A. Allan, W. Alex Marvin, Srinivas Rangarajan, Prodromos Daoutidis
- 10:10 Process alternatives for second generation ethanol production from sugarcane bagasse 854
Felipe F. Furlan, Roberto C. Giordano, Caliane B. B. Costa, Argimiro R. Secchi, John M. Woodley

08:30-10:30 Parallel Session: Monitoring & Estimation (Oral A2.3, T-5.1, 19)

Chair: M. Bhushan, M. A. A. Shoukat Choudhury

08:30	Online models for increased plant availability <i>Friedhelm Steffens, Bernd Pennemann, Franz Beggel, Thomas Bludowski</i>	460
08:50	Improving Data Reliability for Process Monitoring with Fuzzy Outlier Detection <i>Harakhun Tanatavikorn, Yoshiyuki Yamashita</i>	357
09:10	Plantwide Predictive Monitoring of Sulfur Emissions in Tail Gas Treatment Units <i>Eva M. Speelmanns, Francesco Rossi, Andres R. Leon-Garzon, Flavio Manenti</i>	934
09:30	A nonlinear quasi-unknown input observer for the chemostat Droop model <i>Alexander Schaum, Thomas Meurer</i>	216
09:50	Multivariate analysis of industrial scale fermentation data <i>Lisa Mears, Rasmus Nørregård, Stuart M. Stocks, Mads O. Albaek, Gürkan Sin, Krist V. Gernaey, Kris Villez</i>	596
10:10	Parameter estimation and concentration inference for an enzymatic hydrolysis reactor <i>Teresa Lopez-Arenas, Emilio Granada-Vecino</i>	649
08:30-10:30	Parallel Session: Mathematical Programming (Optimisation) I: Numerical Issues (Oral A2.4, T-2.1, 18) <i>Chair: Eva Sorensen, Xavier Joulia</i>	
08:30	Degeneracy Hunter: An Algorithm for Determining Irreducible Sets of Degenerate Constraints in Mathematical Programs <i>Alexander W. Dowling, Lorenz T. Biegler</i>	513
08:50	Deterministic Global Optimization and Transition States <i>Dimitrios Nerantzis, Claire S. Adjiman</i>	620
09:10	Multi-cut multi-column cross decomposition for stochastic mixed-integer linear programming <i>Emmanuel Ogbe, Xiang Li</i>	127
09:30	A robust minimax Semidefinite Programming formulation for optimal design of experiments for model parameterization <i>Belmiro P. M. Duarte, Guillaume Sagnol, Nuno M. C. Oliveira</i>	1006
09:50	Ellipsoidal Arithmetic for Multivariate Systems <i>Mario E. Villanueva, Jai Rajyaguru, Boris Houska, Benoît Chachuat</i>	388
10:10	Optimization Studies through Simulation of a Methanol/Water/Glycerol Distillation Column <i>José Palmeira, João M. Silva, Henrique A. Matos</i>	1060
08:30-10:30	Parallel Session: Pharmaceutical Systems Engineering (Oral A2.5, T-9.3, 20) <i>Chair: Zainuddin A. Manan, Andre Bardow</i>	
08:30	Modeling of Crystallization of Solid Oral Drug Forms in a Dropwise Additive Manufacturing System <i>Elçin İçten, Zoltan K. Nagy, Gintaras V. Reklaitis</i>	672

08:50	Plantwide design and economic evaluation of two Continuous Pharmaceutical Manufacturing (CPM) cases: Ibuprofen and Artemisinin <i>Hikaru G. Jolliffe, Dimitrios I. Gerogiorgis</i>	931
09:10	Optimal Resin Selection for Integrated Chromatographic Separations in High-throughput Screening <i>Songsong Liu, Spyridon Gerontas, David Gruber, Richard Turner, Nigel J. Titchener-Hooker, Lazaros G. Papageorgiou</i>	813
09:30	Model-based optimization of the primary drying step during freeze-drying <i>S��verine T.F.C. Mortier, Pieter-Jan Van Bockstal, Ingmar Nopens, Krist V. Gernaey, Thomas De Beer</i>	382
09:50	PAT for in-depth understanding and process design for crystallization of active pharmaceutical ingredients <i>Thomas B. Hansen, Haiyan Qu</i>	248
10:10	Process-based Method for Reducing Product Losses in Pharmaceutical Manufacturing <i>Hirokazu Sugiyama, Masaaki Ito, Masahiko Hirao</i>	305
09:30 – 10:30	Oral Highlights II (17) <i>Chair: Lei Zhang</i> Posters 242, 256, 277, 696, 894, 1001, 12, 163, 255, 417, 690, 766	
10:30-11:10	Break (Hall A)	
11:10-12:10	Plenary 2 (A11+A12) <i>Chair: Venkat Venkatasubramanian</i>	
11:10	A Multidisciplinary Hierarchical Framework for the Design of Consumer Centered Chemical Products <i>Ka M. Ng, The Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong</i>	952
12:10-13:00	Lunch (Hall A)	
13:00-14:40	Parallel Session: Parameter Estimation & Kinetics (Oral B2.1, T-1.2, A11) <i>Chair: Felipe L��pez-Isunza, Subash Balakrishna</i>	
13:00	Model-based design of experiments for the identification of kinetic models in microreactor platforms <i>Federico Galvanin, Enhong Cao, Noor Al-Rifai, Asterios Gavriilidis, Vivek Dua</i>	433
13:20	Incremental Kinetic Identification based on Experimental data From Steady-state Plug Flow Reactors <i>Nirav Bhatt, Srividhya Visvanathan</i>	921
13:40	Systematic development of kinetic models for systems described by linear reaction schemes <i>Carolina S. Vertis, Nuno M. C. Oliveira, Fernando P. M. Bernardo</i>	996
14:00	Modeling and parameter estimation of coke combustion kinetics in a glycerol catalytic conversion reactor	453

	<i>Minghai Lei, François Lesage, M. Abderrazak Latifi, Serge Tretjak</i>	
14:20	Modeling and Parameter Estimation of Enzymatic Biodiesel Synthesis <i>Priscila S. Sabaini, Thais F.C. Salum, Rossano Gambetta, Fabricio Machado</i>	685
13:00-14:40	Parallel Session: Process Intensification (Oral B2.2, T-4.3, A12) <i>Chair: Khavinet Lourvanij, Alisa Kammafoo</i>	
13:00	Energy efficient bioethanol purification by heat pump assisted extractive distillation in a dividing-wall column <i>Anton A. Kiss, Hao Luo, Costin S. Bildea</i>	710
13:20	Conceptual design of an internally heat-integrated reactive distillation column based on thermodynamic and hydraulic analysis <i>Zixin Lin, Weizhong An, Yawei Xu, Jianmin Zhu</i>	1095
13:40	Computer-aided process analysis of integrated biodiesel processes incorporating reactive distillation and organic solvent nanofiltration <i>Kathrin Werth, Kolja Neumann, Mirko Skiborowski</i>	593
14:00	An Integrated Reactive Distillation Process for Biodiesel Production <i>Eduardo S. Perez-Cisneros, Ricardo Morales-Rodriguez, Mauricio Sales-Cruz, Tomás Viveros-García, Ricardo Lobo-Oehmichen</i>	36
14:20	Alternative Hybrid Liquid-Liquid and Distillation Sequences for the Biobutanol Separation <i>Massimiliano Errico, Eduardo Sanchez-Ramirez, Juan J. Quiroz-Ramírez, Juan G. Segovia-Hernández, Ben-Guang Rong</i>	300
13:00-14:40	Parallel Session: Control Theory and Applications (Oral B2.3, T-5.5, 19) <i>Chair: Jakob K. Huusom, Filip Logist</i>	
13:00	A Decentralised Multi-parametric Model Predictive Control Study for a Domestic Heat and Power Cogeneration System <i>Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos</i>	46
13:20	Model Predictive Control for the Self-Optimized Operation in Wastewater Treatment Plants <i>Mario Francisco, Sigurd Skogestad, Pastora Vega</i>	724
13:40	Multivariable Adaptive Lyapunov Fuzzy Controller for pH neutralisation process <i>Mohd F. Zail, Mohd A. Hussain</i>	535
14:00	Optimised Operation of a Decentralized Wastewater Treatment Plant with Advanced Nitrogen Removal in the Presence of Online Sensor Failures <i>Tatiana Arriaga, Rita Ribeiro, Carla Costa Pinheiro, Helena Maria Pinheiro, Maria do Céu Almeida</i>	352
14:20	Off-Line Tube-Based Robust Model Predictive Control for Uncertain and Highly Exothermic Polymerization Processes <i>Pornchai Bumroongsri, Veerayut Lersbamrungsuk, Soorathep Kheawhom</i>	759

13:00-14:40	Parallel Session: Planning & Scheduling (Oral B2.4, T-7.2, 18) <i>Chair: Gintaras V. (Rex) Reklaitis, Christodoulos A. Floudas</i>	
13:00	On the complexity of production planning and scheduling in the pharmaceutical industry: the Delivery Trade-offs Matrix <i>Samuel Moniz, Ana P. Barbosa-Póvoa, Jorge Pinho de Sousa</i>	119
13:20	Optimal Scheduling of Liquid Drug Product Manufacturing <i>Lukas G. Eberle, Elisabet Capón-García, Martin Senninger, Hirokazu Sugiyama, Andreas Graser, Rainer Schmidt, Konrad Hungerbühler</i>	642
13:40	Planning of a multiproduct pipeline integrating blending and distribution <i>Diovanina Dimas, Valéria V. Murata, Sérgio M. S. Neuro, Susana Relvas, Ana P. Barbosa-Póvoa</i>	108
14:00	Integration of Scheduling and Vessel Routing in Pipeless Plants <i>Munawar A. Shaik, Pulkit Mathur</i>	375
14:20	A Mean Value Cross Decomposition Strategy for Demand-side Management of a Pulping Process <i>Hubert Hadera, Per Wide, Iiro Harjunkoski, Juha Mäntysaari, Joakim Ekström, Guido Sand, Sebastian Engell</i>	435
13:00-14:40	Parallel Session: Energy Systems Design and Scheduling I (Oral B2.5, T-9.5.2, 20) <i>Chair: Brenno C. Menezes, Zdravko Kravanja</i>	
13:00	An Industry View on Improving Energy Efficiency - Developed Methodologies, Applied Tools and Collected Experience <i>Philipp S. Ernst, Arne Braun, Kristian Voelskow, Bastian Mahr, Knud Werner, Fatma van Winssen, Daniela Koelsch, Matthias Boehm</i>	360
13:20	A spatial decomposition procedure for effective solution of energy distribution problems <i>Carl Haikarainen, Frank Pettersson, Henrik Saxén</i>	546
13:40	System Design of Renewable Energy Generation and Storage Alternatives for Large Scale Continuous Processes <i>Oluwamayowa O. Amusat, Paul Shearing, Eric S. Fraga</i>	331
14:00	IGCC Modeling For Simultaneous Power Generation And CO2 Capture <i>Usama Ahmed, Umer Zahid, Chonghun Han</i>	834
14:20	Optimal Scheduling of Air Separation with Cryogenic Energy Storage <i>Qi Zhang, Clara F. Heuberger, Ignacio E. Grossmann, Arul Sundaramoorthy, Jose M. Pinto</i>	207
13:00-14:40	Parallel Session: Reneseng EU-project (Oral B2.6, T-R.1, 17) <i>Chair: Antonis C. Kokossis</i>	
13:00	Production of phthalic anhydride from biorenewables: process design <i>Sara Giarola, Charles Romain, Charlotte K. Williams, Jason P. Hallett, Nilay Shah</i>	249
13:20	Sustainable Process Design under uncertainty analysis: targeting environmental indicators	265

	<i>Carina L. Gargalo, Gürkan Sin</i>	
13:40	Model Integration Using Ontology Input-Output Matching <i>Linsey Koo, Franjo Cecelja</i>	719
14:00	Life Cycle Assessment of biorefinery products based on different allocation approaches <i>Paraskevi Karka, Stavros Papadokonstantakis, Konrad Hungerbühler, Antonis Kokossis</i>	804
14:20	Synthesis and design of multiphase chemical and biochemical reactors <i>Georgios P. Panayiotou, Aikaterini D. Mountraki, Antonis C. Kokossis</i>	1136
14:40-16:00	Elsevier Poster Session 2 (Hall A)	
16:00-17:30	Parallel Keynote Session: Pharma II (Key 2.1, A-8, A11) <i>Chair: Peter M. Harper</i>	
16:00	Modeling and Optimization of Continuous Pharmaceutical Manufacturing Processes <i>Amanda Rogers, Marianthi Ierapetritou, Fernando Muzzio, Rutgers University, USA</i>	646
16:30	Statistical modelling and in-line near-infrared spectrometry in process development of tablet manufacturing <i>Erik Skibsted, Novo Nordisk, Denmark</i>	1148
17:00	Large-scale Multiphase Models for Pharmaceutical Manufacturing Optimization <i>Johannes Khinast, Graz University of Technology, Austria</i>	1134
16:00-17:30	Parallel Keynote Session: Planning & Scheduling II (Key 2.2, A-3, A12) <i>Chair: Ana P. Barbosa-Póvoa</i>	
16:00	Chemical Production Scheduling: From Models to Online Solution Methods <i>Christos Maravelias, Wisconsin University, USA</i>	96
16:30	Crude-oil scheduling technology: moving from simulation to optimization <i>Brenno C. Menezes, Petrobras, Brazil</i>	1149
17:00	Mixed-Integer Fractional Programming: Models, Algorithms, and Applications in Process Operations, Energy Systems, and Sustainability <i>Fengqi You, Northwestern University, USA</i>	1014
16:00-17:30	Parallel Keynote Session: Intelligent Systems (Key 2.3, A-4, 20) <i>Chair: Sachin C. Patwardhan</i>	
16:00	Enterprise Risk Management in Complex Socio-Technical Systems: Challenges and Opportunities <i>Venkat Venkatasubramanian, Columbia University, USA</i>	950
16:30	Cognitive Engineering: Towards Preventing Human Error during Process Operations by Real-Time Monitoring of the Plant Operator <i>Punitkumar Bhavsar, Sweta Parmar, K Madhu, Babji Srinivasan, Rajagopalan Srinivasan, IIT-Gandhinagar, India</i>	479
17:00	Abnormal situation management challenges and opportunities in the big data era <i>Jinsong Zhao, Tsinghua University, China</i>	448
18:00-20:00	Novo Nordisk Reception (invite only)	

Wednesday June 3rd, 2015

08:30-10:30 Parallel Session: Model-based Analysis (Oral A3.1, T-1.5, A11)

Chair: Henrique A. Matos, M. Soledad Diaz

- 08:30 Analysis of the transfer of radical copolymerization systems from semi-batch to continuous plants 193
Thilo Goerke, Sebastian Engell
- 08:50 Behavior of heavy metals during gasification of phytoextraction plants: thermochemical modelling 465
Marwa Saïd, Laurent Cassayre, Jean-Louis Dirion, Ange Nzihou, Xavier Joulia
- 09:10 Global Sensitivity Analysis for a Model of B-Cell Chronic Lymphocytic Leukemia Disease Trajectories 70
Symeon V. Savvopoulos, Ruth Misener, Nicki Panoskaltzis, Efstratios N. Pistikopoulos, Athanasios Mantalaris
- 09:30 Modeling and Sensitivity analysis of a medium-temperature gas cleaning process of biogenous synthesis gas 769
Michaela Fraubaum, Heimo Walter
- 09:50 Data analysis and modelling of a Fluid Catalytic Cracking Unit (FCCU) for an implementation of Real Time Optimization 968
Juan D. Reyes, Adriana L. Rodriguez, Carlos A. M. Riascos
- 10:10 Analyzing and Modeling Ethylene Cracking Process with Complex Networks Approach 555
Fang Zhou, Qiu Tong, Bingzhen Chen

08:30-10:30 Parallel Session: Design of CO₂-based Processes (Oral A3.2, T-4.2, A12)

Chair: Jeffrey J. Siirola, Andreas Bode

- 08:30 CO₂ as feedstock: a new pathway to syngas 112
Flavio Manenti
- 08:50 Carbon capture and utilisation: Application of life cycle thinking to process design 1117
Rosa Cuellar-Franca, Ioanna Dimitriou, Pelayo Garcia-Gutierrez, Rachael H. Elder, Ray W. K. Allen, Adisa Azapagic
- 09:10 Synthetic Methane from CO₂: Dynamic Optimization of the Sabatier Process for Power-to-Gas Applications 378
Ali El Sibai, Liisa Rihko-Struckmann, Kai Sundmacher
- 09:30 Development of sustainable CO₂ conversion processes for the methanol production 323
Kosan Roh, Tuan B. H. Nguyen, Uthaiporn Suriyaphadilok, Jay H. Lee, Rafiqul Gani
- 09:50 CO₂ vs biomass: Identification of environmentally beneficial processes for platform chemicals from renewable carbon sources 884
André Sternberg, Holger Teichgräber, Philip Voll, André Bardow
- 10:10 An Integrated Framework for Controllability Assessment and Solvent Selection in Post-Combustion CO₂ Capture Processes 562
Theodoros Damartzis, Athanasios I. Papadopoulos, Panos Seferlis

08:30-10:30	Parallel Session: Cyber-infrastructure, Informatics & Intelligent Systems (Oral A3.3, T-3.1, 19) <i>Chair: Rajagopalan Srinivasan, Shinji Hasebe</i>	
08:30	Constructing an ontology for physical-chemical processes <i>Heinz A. Preisig</i>	446
08:50	On the Process of Building a Process System Engineering Ontology Using a Semi-Automatic Construction Approach <i>Canan Dombayci, Javier Farreres, Horacio Rodríguez, Edrisi Muñoz, Elisabet Capón-García, Antonio Espuña, Moisès Graells</i>	75
09:10	BiOnto: An Ontology for Biomass and Biorefining Technologies <i>Nikolaos Trokanas, Madeleine Bussemaker, Eirini Velliou, Hella Tokos, Franjo Cecelja</i>	602
09:30	An ontological approach to integration of planning and scheduling activities in the batch process industries <i>Marcela Vegetti, Gabriela Henning</i>	1093
09:50	Enterprise-Wide Scheduling Framework Supported by Knowledge Management <i>Elisabet Capón-García, Edrisi Muñoz, José M. Laínez-Aguirre, Antonio Espuña, Luis Puigjaner</i>	771
10:10	Graphical Processing Unit (GPU) Accelerated Solution of Multi-Dimensional Population Balances Using High Resolution Finite Volume Algorithm <i>Botond Szilagy, Zoltan K. Nagy</i>	500
08:30-10:30	Parallel Session: Mathematical Programming (Optimisation) II: Dynamic Optimisation (Oral A3.4, T-2.2, 18) <i>Chair: Sharifah R. Wan Alwi, Xiangping Zhang</i>	
08:30	Dynamic Modelling and Optimal Design of the Solid-Phase Reactive Chromatographic Separation System for Biomass Saccharification via Acid Hydrolysis <i>Pakkapol Kanchanalai, Matthew J. Realff, Yoshiaki Kawajiri</i>	1015
08:50	Deterministic Global Dynamic Optimisation using Interval Analysis <i>Carlos Perez-Galvan, I. David L. Bogle</i>	477
09:10	Dynamic Multi-Objective Optimization of Batch Chromatographic Separation Processes <i>Anders Holmqvist, Fredrik Magnusson, Bernt Nilsson</i>	527
09:30	An Adaptive Multi-Objective Differential Evolution Algorithm for Solving Chemical Dynamic Optimization Problems <i>Xu Chen, Wenli Du, Feng Qian</i>	529
09:50	An approach to deal with non-convex models in real-time optimization with modifier adaptation <i>Maximiliano Garcia, Juan Pablo Ruiz, Marta Basualdo</i>	955
10:10	A framework for hybrid multi-parametric model-predictive control with application to volatile anaesthesia <i>Ioana Nascu, Richard Oberdieck, Efstratios N. Pistikopoulos</i>	67

08:30-10:30	Parallel Session: Molecular Systems Engineering (Oral A3.5, T-9.1, 20) <i>Chair: Luke E. K. Achenie, Eduardo S. Perez-Cisneros</i>	
08:30	Quantum mechanics simulations from fundamental binding energy to solvent evaluation tool: A case for benzene-cyclohexane separation <i>Narin Lawan, Jirapat Santatiwongchai, Sairoong Muangpil, Attapong Thirasak, Jirut Wattoom, Alisa Kammafoo</i>	1145
08:50	Molecular dynamics simulations with all-atom models for a detailed understanding of protein dye-affinity interaction <i>Juan Liang, Georg Fieg</i>	184
09:10	An Evaluation of Thermodynamic Models for the Prediction of Solubility of Phytochemicals from Orthosiphon Staminues in Ethanol <i>Mohd S. M. Nor, Zainuddin A. Manan, Azizul A. Mustaffa, Chua L. Suan</i>	1092
09:30	Computational Molecular Design of a Water-Compatible Dentin Adhesive System <i>Farhana Abedin, Brock Roughton, Paulette Spencer, Qiang Ye, Kyle V. Camarda</i>	764
09:50	Computer-aided design of solvents for the recovery of a homogeneous catalyst used for alkene hydroformylation <i>Kevin McBride, Kai Sundmacher</i>	558
10:10	Computer-aided Framework for Design of Pure, Mixed and Blended Products <i>Stefano Cignitti, Lei Zhang, Rafiqul Gani</i>	1130
09:30-10:30	Oral Highlights III (17) <i>Chair: Deenesh K. Babi</i> Posters 621, 774, 1021, 481, 1064, 97, 230, 829, 768, 734, 156, 523, 1009	
10:30-11:10	Break (Hall A)	
11:10-12:10	Plenary 3 (A11+A12) <i>Chair: Jay H. Lee</i>	
11:10	Multi-Level Design of Process Systems for Efficient Chemicals Production and Energy Conversion <i>Kai Sundmacher, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany</i>	146
12:10-13:00	Lunch (Hall A)	
13:00-14:40	Parallel Session: Model-based Systems (Oral B3.1, T-1.6, A11) <i>Chair: Arturo Jiménez-Gutiérrez, Chonghun Han</i>	
13:00	A Novel Rigorous Mathematical Programming Approach to Construct Phenomenological Model <i>Vassilios S. Vassiliadis, Yian Wang, Ye Yuancand, Harvey Arellano-Garcia</i>	665
	A framework for a direct exploitation of available information in the online model-based redesign of experiments <i>Riccardo De Luca, Federico Galvanin, Fabrizio Bezzo</i>	55

13:20	A Framework for Modular Modeling of the Diesel Engine Exhaust Gas Cleaning System <i>Andreas Åberg, Thomas K. Hansen, Kasper Linde, Anders K. Nielsen, Rune F. Damborg, Anders Widd, Jens Abildskov, Anker D. Jensen, Jakob K. Huusom</i>	634
13:40	A Modelling, Simulation, and Validation Framework for the Distributed Management of Large-scale Processing Systems <i>Shaghayeg Nazari, Christian Sonntag, Goran Stojanovski, Sebastian Engell</i>	321
14:00	Dynamic Simulation of a Batch Aqueous Two-Phase Extraction Process for α -Amylase <i>Nehal Patel, Daniel G. Bracewell, Eva Sorensen</i>	886
14:20	OsmoseLua - An integrated approach to Energy Systems Integration with LCIA and GIS <i>Min-Jung Yoo, Lindsay Lessard, Maziar Kermani, François Maréchal</i>	920
13:00-14:40	Parallel Session: Generic Methods (Oral B3.2, T-4.6, A12) <i>Chair: David L. Bogle, Ian T. Cameron</i>	
13:00	Optimization of the Integrated Gasification Combined Cycle Using Advanced Mathematical Models <i>Bongani Mvelase, Thokozani Majazi</i>	880
13:20	Design of Hybrid Heat-integrated Configuration for Indirect Reactive Distillation Processes <i>Kuo-Chun Weng, Hao-Yeh Lee</i>	688
13:40	Integrated Design and Control of Semicontinuous Processes Using Mixed Integer Nonlinear Dynamic Optimization <i>Vida Meidanshahi, Thomas A. Adams II</i>	402
14:00	Optimal production of Furfural and DMF from algae and switchgrass <i>Mariano Martín, Ignacio E. Grossmann</i>	99
14:20	Topology optimization for biocatalytic microreactor configurations <i>Inês P. Rosinha, Krist V. Gernaey, John M. Woodley, Ulrich Krühne</i>	647
13:00-14:40	Parallel Session: Abnormal Events Management & Process Safety (Oral B3.3, T-6.1, 19) <i>Chair: Rajagopalan Srinivasan, Jinsong Zhao</i>	
13:00	Leak Identification using Extended Kitanidis-Kalman Filter <i>C. Ganesh, Pushkar Ballal, Mani Bhushan, Sachin C. Patwardhan</i>	961
13:20	Shape Constrained Splines with Discontinuities for Anomaly Detection in a Batch Process <i>Kris Villez, Jonathan Habermacher</i>	744
13:40	Hierarchical Fault Propagation and Control Strategy from the Resilience Engineering Perspective: A Case Study with Petroleum Refining System <i>Jinqiu Hu, Laibin Zhang, Xi Ma, Zhansheng Cai</i>	1085
14:00	Automata Based Test Plans for Fault Diagnosis in Batch Processes <i>Chuei-Tin Chang, Wei-Chung Hsieh</i>	30
14:20	Risk Analysis Applied to Bioethanol Dehydration Processes: Azeotropic Distillation versus Extractive Distillation <i>Adriana Avilés-Martínez, Nancy Medina-Herrera, Arturo Jiménez-Gutiérrez, Medardo</i>	691

Serna-González, Agustín J. Castro-Montoya

13:00-14:40	Parallel Session: Planning & Scheduling (Oral B3.4, T-7.3, 18) <i>Chair: Gabriela P. Henning, Lazaros Papageorgiou</i>	
13:00	Downstream Petroleum Supply Chains Planning under Uncertainty <i>Leão J. Fernandes, Susana Relvas, Ana P. Barbosa-Póvoa</i>	267
13:20	MDP formulation and solution algorithms for inventory management with multiple suppliers and supply and demand uncertainty <i>Joohyun Shin, Jay H. Lee</i>	314
13:40	A Duality-based Approach for Bilevel Optimization of Capacity Expansion <i>Pablo Garcia-Herreros, Pratik Misra, Erdem Arslam, Sanjay Mehta, Ignacio E. Grossmann</i>	1102
14:00	A meta-multiparametric framework: Application to the operation of bio-based energy supply chains <i>Sergio Medina, Ahmed Shokry, Javier Silvente, Antonio Espuña</i>	598
14:20	Process Simulations Supporting a Techno-Economic Framework to Optimize the Biorefinery Supply Chains <i>Sumesh Sukumara, Kwabena Darkwah, Jeffrey R. Seay</i>	801
13:00-14:40	Parallel Session: Energy Systems Design and Scheduling II (Oral B3.5, T-9.5.3, 20) <i>Chair: François Maréchal, Ana Carvalho</i>	
13:00	Financial Considerations in Shale Gas Supply Chain Development <i>Andrés J. Calderón, Omar J. Guerra, Lazaros G. Papageorgiou, Jeffrey J. Siirola, Gintaras V. Reklaitis</i>	666
13:20	Short-term planning of cogeneration power plants: a comparison between MINLP and piecewise-linear MILP formulations <i>Leonardo Taccari, Edoardo Amaldi, Emanuele Martelli, Aldo Bischi</i>	966
13:40	Engineering design of localised synergistic production systems <i>Melissa Y. Leung Pah Hang, Elias Martinez-Hernandez, Matthew Leach, Aidong Yang</i>	723
14:00	Adaptive Management of Renewable Energy Smart Grids Using a Power Grand Composite Curves Approach <i>Damian Giaouris, Athanasios I. Papadopoulos, Panos Seferlis, Simira Papadopoulou, Spyros Voutetakis</i>	917
14:20	Preliminary analysis of systems for integrating solar thermal energy into processes with heat demands <i>Andreja Nemet, Jiří J. Klemeš, Zdravko Kravanja</i>	841
14:40-16:00	Elsevier Poster Session 3 (Hall A)	
16:00-17:30	Parallel Keynote Session: Control (Key 3.1, A-9, A11) <i>Chair: Jakob K. Huusom</i>	
16:00	Towards the integration of process design, control and scheduling: Are we getting closer?	74

	<i>Efsttraios N. Pistikopoulos, Texas A&M University, USA</i>	
16:30	Control of Reaction Systems via Rate Estimation and Feedback Linearization, <i>Diogo Rodrigues, Julien Billeter, Dominique Bonvin, EPFL, Switzerland</i>	166
17:00	Simple rules for economic plantwide control <i>Vladimiro Minasidis, Sigurd Skogestad, NTNU, Norway</i>	967
16:00-17:30	Parallel Keynote Session: PSE for Industry (Key 3.2, A-7, A12) <i>Chair: Konrad Triebeneck</i>	
16:00	Industrial Reflections on Modelling of Fine Chemicals and Seeds Process/Product Design <i>Patrick M. Piccione, Syngenta, UK</i>	85
16:30	A perspective on PSE in fermentation process development and operation <i>Krist V. Gernaey, DTU, Denmark</i>	1057
17:00	NSF Programs and Initiatives in Process Systems Engineering <i>Maria K. Burka, National Science Foundation, USA</i>	1156
16:00-17:30	Parallel Keynote Session: Sustainability, LCA and PSE-tools (Key 3.3, A-5, 20) <i>Chair: Fengqi You</i>	
16:00	Sustainable production and consumption: A decision-support framework based on a systems approach to integrating environmental, economic and social aspects of sustainability <i>Adisa Azapagic, University of Manchester, UK</i>	1120
16.30	Advanced Chemical Manufacturing and Sustainability: A Multidisciplinary Collaboration Approach <i>Yinlun Huang, Wayne State University, USA</i>	776
17:00	Property modelling issues: data, parameter regression and consistency <i>Loïc d'Anterrosches, Céondo, Germany</i>	1157
18:30-01:30	Conference Dinner at Wallman's (doors open at 18:30, seated by 19:00)	

Thursday June 4th, 2015

08:30-10:30	Parallel Session: Modelling & Simulation (Oral A4.1, T-1.3, A11) <i>Chair: Mauricio Sales-Cruz, Ruth Misener</i>	
08:30	Modeling the Fixed-Bed Fischer-Tropsch Reactor in Different Reaction Media <i>Rehan Hussain, Jan H. Blank, Nimir O. Elbashir, Texas A&M University at Qatar, Qatar (keynote)</i>	657
09:10	First-principles model diagnosis in batch systems by multivariate statistical modeling <i>Natascia Meneghetti, Pierantonio Facco, Sean Bermingham, David Slade, Fabrizio Bezzo, Massimiliano Barolo</i>	610
09:30	Mathematical Modeling of an Industrial Delayed Coking Unit <i>Claudio N. Borges, Maria A. Mendes, Rita M. B. Alves</i>	757
09:50	Modelling and Simulation of Pressure Swing Adsorption (PSA) Processes for post-combustion Carbon Dioxide (CO ₂) capture from flue gas <i>George N. Nikolaidis, Eustathios S. Kikkinides, Michael C. Georgiadis</i>	334
10:10	Post-combustion CO ₂ capture with sulfolane based activated alkanolamine solvent <i>Sukanta K. Dash, Bikash K. Mondal, Amar N. Samanta, Syamalendu S. Bandyopadhyay</i>	762
08:30-10:30	Parallel Session: Process Synthesis-Design (Oral A4.2, T-4.5, A12) <i>Chair: Jiří J. Klemeš, Jean-Marc Le Lann</i>	
08:30	Simultaneous Design of Desalination Plants and Distribution Water Network <i>Sebastián Herrera, Luis A. Cisternas, Edelmira D. Gálvez</i>	407
08:50	Inter-process heat integration by coordination among agent systems for heat exchanger network design <i>Naoki Kimura, Tetsuo Kaya, Shintarō Miyamoto, Yoshifumi Tsuge</i>	381
09:10	Improved Design Strategies for Flexible Hydrogen Networks <i>Chuei-Tin Chang, Che-Chi Kuo</i>	26
09:30	Optimal Design of Microfluidic Platforms for Diffusion-Based PCR for “One-Pot” Analysis of Cells <i>Jordan Crow, Luke E. K. Achenie, Chang Lu, Sai Ma, Despina N. Loufakis, Zhenning Cao, Yiwen Chang</i>	408
09:50	A thermodynamic targeting approach for the synthesis of sustainable biorefineries <i>Bilal Patel</i>	617
10:10	The Effect of Charge Composition on the Optimal Operational Parameters of a Batch Extractive Distillation Process <i>Laszlo Hegely, Peter Lang</i>	1013
08:30-10:30	Parallel Session: Batch & Crystallization Process Control (Oral A4.3, T-5.3, 19) <i>Chair: Philip Lutze, Yoshiyuki Yamashita</i>	
08:30	Model-based Observation and Design of Crystal Shapes via Controlled Growth-Dissolution Cycles	597

	<i>Holger Eisenschmidt, Naim Bajcinca, Kai Sundmacher</i>	
08:50	Reaction Monitoring of Cementing Materials through Multivariate Techniques Applied to In Situ Synchrotron X-Ray Diffraction Data <i>Alessandra Taris, Massimiliano Grosso, Mariarosa Brundu, Vincenzo Guida, Alberto Viani</i>	141
09:10	A Performance-Oriented Robust Framework for the Online Model-Based Optimization and Control of (Fed-)Batch Systems <i>Francesco Rossi, Flavio Manenti, Gintaras V. Reklaitis, Guido Buzzi-Ferraris</i>	91
09:30	A real time particle size control framework in non-isothermal antisolvent crystallization processes <i>Navid Ghadipasha, Stefania Tronci, Roberto Baratti, Jose A. Romagnoli</i>	505
09:50	Maximizing Profit of Semi Batch Autocatalytic Esterification Process in the Presence of Disturbance: Application of Cascaded-Conditional Based Online Dynamic Optimization <i>Fakhrony S. Rohman, Suhairi A. Sata, Norashid A. Aziz</i>	443
10:10	Enhancing xylitol bio-production by an optimal feeding policy during fed-batch operation <i>Oscar A. Prado-Rubio, Héctor Hernández-Escoto, Divanery Rodriguez-Gomez, Sarote Sirisansaneeyakul, Ricardo Morales-Rodriguez</i>	973
08:30-10:30	Parallel Session: Mathematical Programming (Optimisation) III (Oral A4.4, T-2.3, 18) <i>Chair: Il Moon, Sten B. Jørgensen</i>	
08:30	An approach to optimize multi-enterprise biofuel supply chains including Nash equilibrium models <i>Ricardo A. Ortiz-Gutiérrez, Sara Giarola, Nilay Shah, Fabrizio Bezzo</i>	192
08:50	Reduced model trust region methods for embedding complex simulations in optimization problems <i>John P. Eason, Lorenz Biegler</i>	409
09:10	Representation of the convex envelope of bilinear terms in a reformulation framework for global optimization <i>Andreas Lundell, Tapio Westerlund</i>	600
09:30	Design of a multi-contaminant water allocation network using multi-objective optimization <i>Sofía D. Almaraz, Marianne Boix, Catherine Azzaro-Pantel, Ludovic Montastruc, Serge Domenech</i>	1050
09:50	A Metaheuristic for Solving Large-Scale Two-Stage Stochastic Mixed 0-1 Programs with a Time Consistent Stochastic Dominance Constraints Risk Averse Strategy <i>Susana Baptista, Ana P. Barbosa-Póvoa, Laureano Escudero, Maria I. Gomes, Celeste Pizarro</i>	737
10:10	Synthesis of inherently safer chemical processes with modular process simulators under the Generalized Disjunctive Programming framework <i>Ruben Ruiz-Femenia, M. Francisca Gómez-Rico, María José Fernández-Torres, Raquel Salcedo Díaz, José Antonio Caballero Suárez</i>	104

08:30-10:30	Parallel Session: Environmental Systems Engineering (Oral A4.5, T-9.6, 20) <i>Chair: Yinlun Huang, Adisa Azapagic</i>	
08:30	Water resources management with dynamic optimization strategies and integrated models of lakes and artificial wetlands <i>Jimena Di Maggio, Vanina Estrada, M. Soledad Diaz</i>	914
08:50	Life Cycle Simulation for an automated Process Plant based on a Two-Dimensional Co-Simulation Approach <i>Mathias Oppelt, Gerrit Wolf, Leon Urbas</i>	65
09:10	A detailed mathematical modelling representation of clean water treatment plants <i>Folashade Akinmolayan, Nina F. Thornhill, Eva Sorensen</i>	892
09:30	Environmental, Societal and Economical optimization of a bioethanol supply chain <i>Carlos Miret, Ludovic Montastruc, Stéphane Negny, Serge Domenech</i>	471
09:50	Simultaneous Design and Planning of CO ₂ Transport Pipeline Network for Carbon Dioxide Capture and Sequestration Project <i>Xiong Zou, Hongguang Dong, Jian Li, Jingqu Wang</i>	466
10:10	A Framework for the Dynamic Modelling of PI Curves in Microalgae <i>Andrea Bernardi, Andreas Nikolaou, Andrea Meneghesso, Benoît Chachuat, Tomas Morosinotto, Fabrizio Bezzo</i>	183
10:30-11:00	Break (Hall A)	
11:00-12:00	Parallel Keynote Session: Industrial Engineering (Key 4.1, B-6, A11) <i>Chair: Bent Sarup</i>	
11:00	Industrially applied PSE for Problem Solving Excellence <i>Antoon ten Kate, AkzoNobel, Holland</i>	150
11:30	The research review for smart plant in petrochemical industry <i>Defang Li, Baihua Jiang, Hansheng Suo, Ya Guo, Petro-Cyber Works Information Tech, China</i>	473
11:00-12:00	Parallel Keynote Session: Bioprocess Design (Key 4.2, B-4, A12) <i>Chair: Krist V. Gernaey</i>	
11:00	Process Technology Licensing: An Interface of Engineering and Business <i>Andreas Bode, BASF, Germany</i>	954
11:30	Economic evaluation of large scale bioprocesses - technical and business issues <i>J. Villadsen, J. M Woodley, DTU, Denmark</i>	1150
11:00-12:00	Parallel Keynote Session: Process Intensification (Key 4.3, B-3, 20) <i>Chair: Mario R. Eden</i>	
11:00	PSE Tools for Process Intensification <i>Philip Lutze, TU-Dortmund, Germany</i>	63
11:30	Systematic Design Procedure of Micro Chemical Plants <i>Shinji Hasebe, Kyoto University, Japan</i>	1124

12:00-13:00	Lunch (Hall A)	
13:00-14:00	Parallel Keynote Session: Modelling (Key 5.1, B-5, 18) <i>Chair: Andreas A. Linninger</i>	
13:00	A PSE approach to patient-individualized physiologically based pharmacokinetic modeling <i>Roberto Andrea Abbiati, Gaetano Lamberti, Anna Angela Barba, Mario Grassi, Davide Manca, Politecnico de Milano, Italy</i>	631
13:30	Structure Based Drug Discovery and Design from Optimization Perspective: Observations, Applications and Result <i>Metin Turkay, Koc Univ, Turkey</i>	1123
13:00-14:00	Parallel Keynote Session: Optimization (Key 5.2, B-1, 19) <i>Chair: Masahiko Hirao</i>	
13:00	Steam System Optimization at Mitsubishi Chemical Corporation Kashima Site <i>Toshiharu Morishita, Mitsubishi Chem Corp, Japan</i>	155
13:30	Advances in Chemical Reaction Analysis and Optimization <i>Subash Balakrishna, Optience, USA</i>	71
13:00-14:00	Parallel Keynote Session: Process Design (Key 5.3, B-2, 20) <i>Chair: Antoon ten Kate</i>	
13:00	Process Systems Engineering Approaches to Multi-Scale Chemical Product Design <i>Sarah E. Davis, Robert H. Herring III, Christopher B. Roberts, Mario Richard Eden, Auburn University, USA</i>	493
13:30	New paradigm of chemical process design: from molecule to system <i>Xiangping Zhang, Suojiang Zhang, Xin Zhang, Ying Huang, IPE, CAS, China</i>	190
14:05-14:50	Plenary 4 (A11+A12) <i>Chair: Rafiqul Gani</i>	
14:05	Highlights and New Directions for PSE <i>Gintaras V. (Rex) Reklaitis, Purdue University, West Lafayette, USA</i>	1151
14:50-15:20	Closing session (A11+A12) Including presentations of the next ESCAPE-26 and PSE-2018; awards	
15:20-15:50	Farewell Goodbye with Coffee, tea & cakes	

Elsevier Poster Session 1 (Hall A) – Monday 09:00-18:00

Panel: *Mauricio Sales-Cruz, Fernando L. P. Pessoa, Valentin Pleşu, Bent Sarup, Natalia Menshutina*
(105 Posters)

T-0: PSE-CAPE & Education

P1-1	ORAL HIGHLIGHTS I Experiences in using Operator and 3D Immersive Training Simulators in the Undergraduate Chemical Engineering Curriculum Richard Turton, Debangsu Bhattacharyya	385
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