MONDAY, May 28, 2007

Room	***CONSTANTA***
08:00	***Registration of participants***
08:30	Opening Session
Co-chairmen	*Valentin Pleşu, Paul Ş. Agachi*
09:10	**PLENARY LECTURE** T0-649 Process Systems Engineering and CAPE – What Next? *Rafiqul Gani, Ignacio E. Grossmann*
10:00	Coffee Break

	Session 1 **T1 - MODELLING IN CAPE – NEW HORIZONS**	**Session 2** **T2 - PRODUCTS AND PROCESSES DESIGN FUNDAMENTALS**
Room	***CONSTANTA***	***Salon A***
Co-chairmen	*Christodoulos Floudas, Peter Glavič*	*Jean-Marc LeLann, Paul Barton*
10:20	**KEYNOTE LECTURE** T1-58 State-of-the Art in Short-Term, Medium-Term, and Reactive Scheduling for Large-Scale Batch and Continuous Processes, *Christodoulos Floudas*	**KEYNOTE LECTURE** T2-648 - Management of Innovation and Process System Engineering, *Jean-Marc LeLann, Stephane Negny*
11:00	T1-268 - Neural networks for modelling material thermostability, *Cătălin Lisa, Silvia Curteanu, Gabriela Lisa, Daniela Apreutesei*	T2-173 - Design and Control of PFR-Separation-Recycle Systems with Simultaneous Exothermic and Endothermic Reactions, *Costin S. Bildea, Klaas Steur, Alexandre C. Dimian*
11:20	T1-354 - A Computer Aided Framework for Prediction of Properties of Organic Systems, *Hugo E. González Villalba, Jens Abildskov, Rafiqul Gani*	T2-242 - Decision Process Modeling in Chemical Engineering Design, *Manfred Theißen, Wolfgang Marquardt*
11:40	T1-454 - Automatic Generation of Combustion Mechanisms, *Sauro Pierucci, Eliseo Ranzi*	T2-128 – Integrated Product and Process Design Approach for Rationalization of Food Products, *Cristhian Almeida-Rivera, Puneet Jain, Solke Bruin, Peter Bongers*
12:00	T1-521 - Combining Reaction Kinetics to the Multi-phase Gibbs Energy Calculation, *Pertti Koukkari, Risto Pajarre*	T2-231 - Model Based Design of Polymer Product, *Dulce C.M. Silva, Nuno M.C. Oliveira*

12:20	Presentation of ESCAPE 18
12:40	Lunch Champions/Cupola Restaurants

MONDAY, May 28, 2007

		Room
		08:00
		08:30
		09:10
	Coffee Break	10:00
Session 3 **T3 - OPTIMISATION AND OPTIMAL PROCESS CONTROL AND OPERATION**	**Session 4** **T5 - PROCESS INTEGRATION AND SUSTAINABLE DEVELOPMENT**	
Salon B	***Salon C***	Room
Johan Grievink, Georges Heyen	*Robin Smith, Ferenc Friedler*	Co- chairmen
T3-115 - Optimal Sizing of Production Units for Goods Subject to Stochastic Demand, *Belmiro P.M. Duarte, Nuno M.C. Oliveira, Jorge S. Mariano*	T5-122 - Integration and Resources Management of Small and Medium Enterprises, *Toshko Zhelev, Bernadette O'Regan, Richard Moles*	10:20
T3-424 - Analyzing the Relationship between Manufacturing Lead-times and Line Flexibility – the Line Flexibility Model, *Marlene Klompenhouwer, Zofia Lukszo, Frank Janssen*	T5-158 - A Chemical Process Design Framework Including Different Stages of Environmental, Health and Safety (EHS) Assessment, *Hirokazu Sugiyama, Ulrich Fischer, Masahiko Hirao, Konrad Hungerbühler*	10:40
T3-147 - Generic vs. Engineered Evolutionary Algorithms in Batch Scheduling with Recourse, *Guido Sand, Thomas Tometzki, Jochen Till, Maren Urselmann, Michael Emmerich, Sebastian Engell*	T5-251 - Application of Life Cycle Assessment to the Structural Optimization of Process Flowsheets, *Gonzalo Guillén-Gosálbez, José A. Caballero, Laureano Jiménez Esteller, Mamdouh Gadalla*	11:00
T3-195 - Genetic Algorithms for the Scheduling of Multiproduct Batch Plants within Uncertain Environment, *Antonin Ponsich, Anna Bonfill, Antonio Espuña, Catherine Azzaro-Pantel, Serge Domenech, Luc Pibouleau*	T5-443 - Modelling and Numerical Simulation of Ice Slurry Storage Tank, *Denis Flick, Christophe Doursat, Mohamed Ben Lakhdar*	11:20
T3-206 - A Bi-level Decomposition Scheme for the Integration of Planning and Scheduling in Parallel Multi-Product Batch Reactors, *Muge Erdirik-Dogan, Ignacio E. Grossmann, John Wassick*	T5-562 - Business Model of Plant Maintenance for Lifecycle Safety, *Tetsuo Fuchino, Masazumi Miyazawa, Yuji Naka*	11:40
T3-262 - Modelling an Ice Cream Factory for de-Bottlenecking, *Peter Bongers, Bas Bakker*	T5-580 - Minimization of Life Cycle CO_2 Emissions in the Operation of a Steam and Power Plant, *Ana Maria Eliceche, Pablo E. Martinez*	12:00
		12:20
Lunch Champions/Cupola Restaurants		12:40

MONDAY, May 28, 2007

	Session 5 T5 - PROCESS INTEGRATION AND SUSTAINABLE DEVELOPMENT	Session 6 T3 - OPTIMISATION AND OPTIMAL PROCESS CONTROL AND OPERATION
Room	***CONSTANTA***	***Salon A***
Co-chairmen	*Jiří Klemeš, Ana Maria Eliceche*	*Sorin Costin Bildea, Efstratios Pistikopoulos*
14:00	**KEYNOTE LECTURE** T5-453 - Integration of Process Site Utility Systems, *Robin Smith*	**KEYNOTE LECTURE** T3-38 - Parametric Programming & Control: From Theory to Practice, *Efstratios N. Pistikopoulos, Michael C. Georgiadis, Vivek Dua*
14:40	T5-370 - Biodiesel Production by Integrated Reactive-Separation Design, *Anton A. Kiss, Alexandre C. Dimian, Gadi Rothenberg*	T3-130 - Optimal Supply Chain Redesign using Genetic Algorithm, *Pavan Kumar Naraharisetti, Iftekhar A. Karimi, Rajagopalan Srinivasan*
15:00	T5-385 - Methodology for the Optimal Thermo-economic, Multi-objective Design of Thermochemical Fuel Production from Biomass, *Martin Gassner, François Maréchal*	T3-233 - Integrating Process Operations and Finances for the Optimal Design of Chemical Supply Chains, *José Miguel Laínez, Gonzalo Guillén-Gosálbez, Mariana Badell, Antonio Espuña, Luis Puigjaner*
15:20	T5-43 - Integration of the bio-Ethanol Process in a Network of Facilities for Heat and Power Production from Renewable Sources using Process Simulation, *Walter Wukovits, Martin Pfeffer, Bettina Liebmann, Anton Friedl*	T3-489 - Optimisation of MSF Desalination Process for Fixed Water Demand using gPROMS, *Md Sowgath Tanvir, Iqbal Mohammed Mujtaba*
15:40	T5-632 - NLP Optimization of a Methanol Plant by using H_2 co-Product in Fuel Cells, *Anita Kovač Kralj, Peter Glavič*	T3-615 - Generic Modelling and Simulation of Stock Levels in Supply Chains, *Edric Margono, Nouri Samsatli, Nilay Shah*
16:00	Coffee Break	

MONDAY, May 28, 2007

Session 7 **T2 - PRODUCTS AND PROCESSES DESIGN FUNDAMENTALS**	**Session 8** **T1 - MODELLING IN CAPE - NEW HORIZONS**	
Salon B	***Salon C***	Room
Alexandre Dimian, Andrzej Kraslawski	*Gintaras Reklaitis, Günter Wozny*	Co- chairmen
T2-189 - A Mathematical Programming Approach to the Analysis, Design and Scheduling of Offshore Oilfields, *Richard J. Barnes, Antonis Kokossis*	T1-108 - The Solution of DAE Systems by a Numerically Robust and Efficient Solver, *Davide Manca, Guido Buzzi-Ferraris*	14:00
T2-567 - Pressure-driven Steady-State Simulation of Oilfield Infrastructure, *Pascal Floquet, Xavier Joulia, Alain Vacher, Martin Gainville, Michel Pons*	T1-109 - A Novel Approach to Predicting the Behavior of Arbitrary Particulate Mixtures under Vibration, *Xiaodong Jia, Richard Caulkin, Mike Fairweather, Richard A Williams*	14:20
T2-627 - A Production Allocation Framework for Natural Gas Production Systems, *Paul I. Barton, Ajay Selot*	T1-27 - *ReDrop* – A General Method for Solving Drop-population Balances with an Arbitrary Number of Property Variables, *Murat Kalem, Andreas Pfennig*	14:40
T2-111 - Heat Integration of Ammonia Cooling Unit into the Purification Process of Fats and Oils, *Tovazhnyanskyy Leonid, Kapustenko Petro, Ulyev Leonid, Boldyrev Stanislav, Garev Andrey*	T1-408 - Spectral Galerkin Method in the Study of Mass Transfer in Laminar and Turbulent Flows, *Tudor Boaca, Ioana Boaca*	15:00
T2-478 - Steady-state Optimisation of the Leaching Process at Kwinana Nickel Refinery, *Travis M. Woodward, Parisa A. Bahri*	T1-463 - An Efficient Solution Method for the MINLP Optimization of Chemical Processes, *Korbinian Kraemer, Sven Kossack, Wolfgang Marquardt*	15:20
T2-556 - A Method for Quick Evaluation of Stepwise Plant Expansion Scenarios in the Chemical Industry, *Jan Oldenburg, Martin Schlegel, Jan Ulrich, Thieu-Luan Hong, Bernhard Krepinsky, Georg Grossmann, Axel Polt, Heinrich Terhorst, Joost-Willem Snoeck*	T1-586 - Fuzzy Logic Model for the Performance Benchmarking of Sugar Plants by considering Best Available Techniques, *Damjan Krajnc, Peter Glavič*	15:40
Coffee Break		16:00

MONDAY, May 28, 2007

	Session 9 **T5 - PROCESS INTEGRATION AND SUSTAINABLE DEVELOPMENT**	**Session 10** **T4 - SYSTEMS BIOLOGY AND BIOLOGICAL PROCESSES**
Room	***CONSTANTA***	***Salon A***
Co-chairmen	*Michael Narodoslawsky, Truls Gundersen*	*Elmar Heinzle, Gheorghe Maria*
16:20	**KEYNOTE LECTURE** T5-88 – The Ecological Impact of the Sugar Sector- Aspects of the Change of a Key Industrial Sector in Europe, *Gernot Gwehenberger, Michael Narodoslawsky*	**KEYNOTE LECTURE** T4-593 – Analysis and Design of Metabolic Networks – Experiments and Computer Simulation, *Elmar Heinzle, Tae Hoon Yang, Rahul Deshpande*
17:00	T5-142 – Novel Energy Saving Technologies Evaluation Tool, *Jiří Klemeš, Igor Bulatov, Jaap Koppejan, Ferenc Friedler, Jens Hetland*	T4-175 – De Novo Peptide Identification via Mixed-Integer Linear Optimization and Tandem Mass Spectrometry, *Peter A. DiMaggio Jr., Christodoulos A. Floudas*
17:20	T5-271 – Rate-based Design of Integrated Distillation Sequences, *Ivo Mueller, Oana-Marlena Penciu, Eugeny Y. Kenig, Maria Gavrilescu*	T4-2 – Development and Implementation of a non-Parametric/Metabolic Model in the Process Optimisation of PHA Production by Mixed Microbial Cultures, *João Miguel Lopes Dias, Paulo Lemos, Luísa Serafim, Adrian Oehmen, Maria A. M. Reis, Rui Oliveira*
17:40	T5-329 – Process Integration under Size Constraints: Logistical Fuels for Mobile Applications, *Jennifer L. Wilder, Rose M. Hanks, Kristin H. McGlocklin, Norman E. Sammons Jr., Mario R. Eden, Bruce J. Tatarchuk*	T4-378 – Identifying Synergistically Switching Pathways for Multi-Product Strain Improvement using Multiobjective Flux Balance Analysis, *Suresh Selvarasu, Dong-Yup Lee, Iftekhar A. Karimi*
19:30	W.A. Mozart Festive Concert with Bucharest Physicians' Orchestra at Romanian Athenaeum	

MONDAY, May 28, 2007

Session 11 **T3 – OPTIMISATION AND OPTIMAL PROCESS CONTROL AND OPERATION**	**Session 12** **T1- MODELLING IN CAPE – NEW HORIZONS**	
Salon B	***Salon C***	Room
Jaroslav Pekar, I.D.L. Bogle	*Xavier Joulia, Heinz Preisig*	Co- chairmen
KEYNOTE LECTURE T3-655 Advanced Process Management for Power and Industrial Energy, *Valdimir Hlavena, Jaroslav Pekar*	T1-144 - Modeling of a Three-phase Industrial Batch Reactor using a Hybrid First -principles Neural-network Model, *Levente L. Simon, Ulrich Fischer, Konrad Hungerbühler, Stavros Papadokonstantakis*	16:20
	T1-161 - Air Quality Prediction in Uberlândia, Brazil, Using Linear Models and Neural Networks, *Taisa S. Lira, Marcos A. S. Barrozo, Adilson J. Assis*	16:40
T3-253 - Optimal Control of a Hybridoma Bioreactor. Changes Induced by Considering by-Products in the Objective Function, *Irina Dana Ofiteru, Alexandru Woinaroschy, Vasile Lavric*	T1-21 - Systematic Qualitative Experimental Design Based upon Identifiability Analysis, *Florin Paul Davidescu, Henrik Madsen, Sten Bay Jørgensen*	17:00
T3-210 - Robust Dynamic Programming via Multi-Parametric Programming, *Nuno P. Faísca, Kostas I. Kouramas, Pedro M. Saraiva, Berç Rustem, Efstratios N. Pistikopoulos*	T1-390 - Optimal Experimental Design Based on Global Sensitivity Analysis, *Maria Rodriguez-Fernandez, Sergei Kucherenko, Costas Pantelides, Nilay Shah*	17:20
T3-143 - Optimal Temperature Control of an Industrial Batch Reactor with Regard to Swelling, *Levente L. Simon, Marina Introvigne, Ulrich Fischer, Konrad Hungerbühler*	T1-456 - Incremental identification of transport phenomena in wavy films, *Maka Karalashvili, Sven Groß, Adel Mhamdi, Arnold Reusken, Wolfgang Marquardt*	17:40
W.A. Mozart Festive Concert with Bucharest Physicians' Orchestra at Romanian Athenaeum		19:30

TUESDAY, May 29, 2007

Room	***CONSTANTA***
08:00	***Registration of participants***
Co-chairmen	*Lorenz Biegler, Gintaras Reklaitis*
09:00	**PLENARY LECTURE** T0-653 - Perspectives for Process Systems Engineering - a Personal View from Academia and Industry, *Karsten-Ulrich Klatt, Wolfgang Marquardt*
09:45	**PLENARY LECTURE** T0-650 - Reactive and Hybrid Separations of Chemicals and Bioactive Substances: Modeling and Optimization, *Andrzej Górak*
10:30	Coffee Break

	Session 1 **T1 - MODELLING IN CAPE - NEW HORIZONS**	**Session 2** **T3 - OPTIMISATION AND OPTIMAL PROCESS CONTROL AND OPERATION**
Room	***CONSTANTA***	***Salon A***
Co-chairmen	*Wollfgang Marquardt, Davide Manca*	*Ernesto Martinez, Sebastian Engel*
10:50	**KEYNOTE LECTURE** T1-641 - Perspectives on Process Systems Engineering R&D in Support of Pharmaceutical Product/ Process Development and Manufacturing, Gintaras V. Rex Reklaitis	**KEYNOTE LECTURE** T3-638 - Large-scale Nonlinear Programming: An Integrating Framework for Enterprise-Wide Dynamic Optimization, *Lorenz T. Biegler*
11:30	T1-155 - An Overview of the Interoperability Roadmap for COM/.NET-Based CAPE-OPEN, *William M. Barrett, Michel Pons, Lars von Wedel, Bertrand Braunschweig*	T3-112 - Analysis of Design and Control of Reactive Thermally Coupled Distillation Sequences, *Fabricio Omar Barroso-Muñoz, Salvador Hernández, Babatunde Ogunnaike*
11:50	T1-272 - A Study on Hydrodynamics and Mass Transfer of Moving Liquid Layers Using Computation Fluid Dynamics, *Theodoros Atmakidis, Eugeny Y. Kenig*	T3-432 - Control of Temperature Profile in the Injection Molding Process for Part Consistency *Brian Bullecks, Samantha Burnham, Gregory Campbell, Raghunathan Rengaswamy, Ravi Kumar Mandela*
12:10	T1-392 - CFD Modelling of Trickle-Bed Reactors for Wastewater Treatment, *Rodrigo Lopes and Rosa M. Quinta-Ferreira*	T3-577 - Robust implementation of optimal strategies accounting for controller performance and uncertainty, *Tilman Barz, Harvey Arellano-Garcia, Günter Wozny*
12:30	Lunch Champions/Cupola Restaurants	

TUESDAY, May 29, 2007

		Room
		08:00
		09:00
		09:45
Coffee Break		10:30
Session 3 **T2 - PRODUCTS AND PROCESSES DESIGN FUNDAMENTALS**	**Session 4** **T5 - PROCESS INTEGRATION AND SUSTAINABLE DEVELOPMENT**	
Salon B	***Salon C***	Room
Alexandre Dimian, Ana Paula Barbosa-Póvoa	*Sauro Pierucci, Toshko Zhelev*	Co-chairmen
T2-334 - A Hierarchal Approach based on Reverse Design Algorithm for Simultaneous Design and Analysis of Product and Processes, *Vipasha Soni, Jens Abildskov, Gunnar Jonsson, Rafiqul Gani*	T5-203 - Integration of Fuel Cells into Combined Power Cycles, *Petar Varbanov, Jiří Klemeš, Ferenc Friedler*	10:50
T2-371 - Overcoming Equilibrium Limitations in Reactive Dividing-Wall Columns, *Anton A. Kiss, Hans Pragt, Cornald van Strien*	T5-275 - Methodology and Software for Prediction of Cogeneration Steam Turbines Performances, *George Darie, Horia Ionuț Petcu*	11:10
T2-471 - Influence of Brine Spray System on the Thermal Salt Recrystallisation Process by Dynamic Simulation, *Raquel D. Moita, Henrique A. Matos, Cristina Fernandes, Clemente P. Nunes, Mário J. Pinho*	T5-36 - Optimization of Electricity / Hydrogen Cogeneration from Generation IV Nuclear Energy Systems, *Adrien Gomez, Catherine Azzaro-Pantel, Luc Pibouleau, Serge Domenech, Christian Latgé, Patrick Dumaz, David Haubensack*	11:30
T2-541 - A Model of Grinding-Classification Circuit Including Particles Size Distribution and Liberation of Material: Application to the Design and Retrofit of Flotation Circuit, David A. Méndez, Edelmira D. Gálvez, Luis A. Cisternas	T5-623 - A new Process Synthesis Methodology utilizing Pressure Exergy in Subambient Processes, *Audun Aspelund, Truls Gundersen*	11:50
T2-548 - Ant Colony Optimization: A Leading Algorithm in Future Optimization of Chemical Processes *Farzaneh Jalalinejad, Farhang Jalali-Farahani, Navid Mostoufi, Rahmat Sotudeh-Gharebagh*	T5-631 - NLP Optimization of Gas Turbine Including Experimental Catalyst Conversion Data in Methanol Plant, *Anita Kovač Kralj, Peter Glavič*	12:10
Lunch Champions/Cupola Restaurants		12:30

TUESDAY, May 29, 2007

Room ***Salon D***

14:00 **POSTER SESSION**

	Session 5 **T5 - PROCESS INTEGRATION AND SUSTAINABLE DEVELOPMENT**	**Session 6** **T1 - MODELLING IN CAPE - NEW HORIZONS**
Room	***CONSTANTA***	***Salon A***
Co-chairmen	*Luis Puigjaner, Jelenka Savkovic-Stevanovic*	*Guido Buzzi-Ferraris, Heinz Preisig*
15:00	T5-140 – Risk Assessment of the Respiratory Health Effects Due to Air Pollution and Meteorological Factors in a Population from Drobeta Turnu Severin, Romania, *Cristina Petrescu, Uwe Schlink, Matthias Richter, Oana Suciu, Romanița Ionovici, Olf Herbarth*	T1-654 – Still Crossing the Chasm: Chemical Engineering Modeling in Drug Discovery and Development *Andrei A. Zlota*
15:20	T5-97 – Modeling and Verification of Control Logics in Safety Instrumented System for Chemical Industrial Processes *Jinkyung Kim, Younghee Lee, Il Moon*	T1-96 – Row by row simulation of heat recovery steam generators: comparing different types of initialization as well as the LMTD and ε-NTU simulation methods, *Marie-Noëlle Dumont, Georges Heyen*
15:40	T5-150 – An Agent-based Model for Water Quality Control, *Constantin Nichita, Mihaela Oprea*	T1-465 – Basis for Bond-graph Modeling in Chemical Engineering, *Françoise Couenne, Christian Jallut, Laurent Lefèvre, Yann Le Gorrec, Bernhard Maschke*
16:00	Coffee Break	

TUESDAY, May 29, 2007

CONSTANTA		Room
EURECHA SESSION		14:00
Session 7 **T1 – MODELLING IN CAPE – NEW HORIZONS**	**Session 8** **T5 – PROCESS INTEGRATION AND SUSTAINABLE DEVELOPMENT**	
Salon B	***Salon C***	Room
Srinivasan Rajagopalan, Manuel Rodriguez	*Zdravko Kravaja, Peter Glavič*	Co- chairmen
T1-168 - Control Loop Performance Assessment Using Ordinal Time Series Analysis, *Ernesto Martínez, César de Prada*	T5-588 - Absorption with Chemical Reaction: Evaluation of Rate Promoters Effect on CO_2 Absorption in Hot Potassium Carbonate Solutions, *Teodor Todinca, Cristian Tănasie, Tobias Pröll, Adina Căta*	15:00
T1-191 - On the Systematic Extraction of Knowledge in Process Synthesis and Chemical Process Design, *Claudia Labrador-Darder, Antonis C. Kokossis, Patrick Linke*	T5-637 - DME Synthesis via Catalytic Distillation: Experiments and Simulation, *Marco Di Stanislao, Alberto Malandrino, Renata Patrini, Carmen Pirovano, Aurora Viva, Elisabetta Brunazzi*	15:20
T1-202 - Data-Driven Decision Support and its Applications in the Process Industries, *Petr Stluka, Karel Mařík*	T5-72 - Plate and Spiral Heat Exchangers for Wet Phosphoric Acid Production Processes, *Petro Kapustenko, Gennadiy Khavin, Oleksandr Perevertaylenkor, Olga Arsenyeva*	15:40
Coffee Break		16:00

TUESDAY, May 29, 2007

	Session 9 **T1 - MODELLING IN CAPE - NEW HORIZONS**	**Session 10** **T2 - PRODUCTS AND PROCESSES DESIGN FUNDAMENTALS**
Room	***CONSTANTA***	***Salon A***
Co-chairmen	*Antonis Kokossis, Bertrand Braunschweig*	*Efstratios N. Pistikopoulos, Vasile Lavric*
16:20	T1-260 – Data Reconciliation of Streams with Low Concentrations of Sulphur Compounds in Distillation Operation, *Kaj Jakobsson, Fredrik Roswall, Kari Keskinen, Juhani Aittamaa*	T2-348 – Model-based Hybrid Reaction-Separation Process Design, *Piotr Tomasz Mitkowski, Gunnar Jonsson, Rafiqul Gani*
16:40	T1-93 - Using Moving Finite Elements Method to Solve Population Balance Equations Comprising Breakage Terms, *Belmiro P.M Duarte, Cristina M.S.G. Baptista*	T2-363 – Hybrid Modelling Methodology to Implement Chemical Process Models as Phenomena-based Modules, *Jorge A. Arizmendi-Sánchez, Paul N. Sharratt*
17:00	T1-388 – A Deliverable from CO-LaN to CAPE-OPEN Developers and Users: the CAPE-OPEN Logging and Testing Tool (COLTT), *Michel Pons, Peter Banks, Bertrand Braunschweig*	T2-488 – Multi-Objective Design of Reactive Distillation, *Rui M. Filipe, Steinar Hauan, Henrique A. Matos, Augusto Q. Novais*
17:20	T1-428 – Population balance model of heat transfer in gas-solid turbulent fluidization, *Zoltán Süle, Csaba Mihálykó, Béla G. Lakatos*	T2-491 – A Methodology for the Approximate Stochastic Synthesis of Flexible Chemical Processes, *Zorka Novak Pintarič, Zdravko Kravanja*
17:40	T1-467 – Debugging for Equation-Oriented CAPE Tools, *Rafael de Pelegrini Soares, Argimiro R. Secchi*	T2-0 – Reactive Distillation Process Analysis in Dividing Wall Column, *Gheorghe Bumbac, Alexandra Elena Pleşu, Valentin Pleşu*
19:30	ESCAPE17 BANQUET – Parliament House - “Take Ionescu Hall”	

TUESDAY, May 29, 2007

Session 11 **T3 – OPTIMISATION AND OPTIMAL PROCESS CONTROL AND OPERATION**	**Session 12** **T4 – SYSTEMS BIOLOGY AND BIOLOGICAL PROCESSES**	
Salon B	***Salon C***	Room
Lorenz Biegler, Henrique A. Matos	*Iftekhar Karimi, Frank Allgöwer*	Co- chairmen
T3-333 - On the Application of Model Reduction to Plantwide Control, *Bogdan Dorneanu, Costin Sorin Bildea, Johan Grievink*	T4-182 - A New De Novo Approach for Optimizing Peptides that Inhibit HIV-1 Entry, *Ho Ki Fung, Christodoulos A. Floudas, Martin S. Taylor, Robert F. Siliciano*	16:20
T3-411 - Iterative Controller Tuning for Processes with Fold Bifurcations, *Jakob Kjøbsted Huusom, Niels Kjølstad Poulsen, Sten Bay Jørgensen*	T4-212 - Modelling the Inhibition Activity on Carbonic Anhydrase I of Some Substituted Thiadiazole- and Thiadiazoline-Disulfonamides: Integration of Structure Information, *Sorana-Daniela Bolboacă, Lorentz Jäntschi*	16:40
T3-455 - Comparison between Different Control Approaches of the UOP Fluid Catalytic Cracking Unit, *Mircea V. Cristea, Paul Ş. Agachi*	T4-426 - Controlled Release of Drugs from Polymeric Devices, *Vivek Dua*	17:00
T3-48 - Iterative Batch-to-Batch Control of Particle Size Distribution in Semi-Batch Emulsion Polymerisation, *Charles D. Immanuel, Ying Wang, Nicola Bianco*	T4-621 - QSAR Analysis of 1,4-Dihydropyridine Calcium Channel Antogonists, *Pınar Kahraman, Metin Türkay*	17:20
T3-7 - Extremum-seeking Control of Redox Processes in Wastewater Chemical Treatment Plants, *Ernesto Martínez*		17:40
ESCAPE17 BANQUET – Parliament House - “Take Ionescu Hall”		19:30

WEDNESDAY, May 30, 2007

Room	***CONSTANTA***	
08:00	***Registration of participants***	
Co-chairmen	*Rafiqul Gani, Christodoulos Floudas*	
09:00	**PLENARY LECTURE** T0-651 - Crystal Engineering for Product and Process Design, *Michael F. Doherty*	
09:45	**PLENARY LECTURE** T0-652 - Among the Trends for a Modern Chemical Engineering: CAPE an Efficient Tool for Process Intensification and Product Design and Engineering, Jean-Claude Charpentier	
10:30	Coffee Break	
	Session 1 **T2 - PRODUCTS AND PROCESSES DESIGN FUNDAMENTALS**	**Session 2** **T4 - SYSTEMS BIOLOGY AND BIOLOGICAL PROCESSES**
Room	***CONSTANTA***	***Salon A***
Co-chairmen	*Xavier Joulia, Mario Eden*	*Gintaras Reklaitis, Il Moon*
10:50	**KEYNOTE LECTURE** T2-100 - Renewable Raw Materials: Chance and Challenge for Computer-Aided Process Engineering, *Alexandre C. Dimian*	**KEYNOTE LECTURE** T4-647 - Live & let die - A Systems Biology View on Cell Death, *Thomas Eißing, Madalena Chaves, Frank Allgöwer*
11:30	T2-50 - Identifying Applicability Domains for Quantitative Structure Property Relationships, *Mordechai Shacham, Neima Brauner, Georgi St. Cholakov, Roumiana P. Stateva*	T4-528 - Increasing the Predictivity of Kinetic Models for High-Cell-Density Cultivations, *Harvey Arellano-Garcia, Anja Drews, Udo Schubert, Günter Wozny, Matthias Kraume*
11:50	T2-575 - Reliable Nonlinear Parameter Estimation in Predicting the Activity Coefficients for Complex Hydrocarbon Mixtures, *Diethmar Richter, Nicolas Cruz Bournazou, Harvey Arellano-García, Holger Thielert, Günter Wozny*	T4-425 - Modeling of the fermentation in an internal loop airlift reactor, *Ivan Sikula, Martin Juraščík, Jozef Markoš*
12:10	T2-110 - Numerical investigation of a dynamical model for emulsion pseudo-homopolymerization *Thibaut Besson, Cheng-Zhong Xu, Nida Sheibat-Othman, Hassan Hammouri*	T4-90 - Modular and Multilayer Modeling – Application to Biological Processes, *Michael B. Cutlip, Mordechai Shacham*
12:30	Lunch Champions/Cupola Restaurants	

WEDNESDAY, May 30, 2007

		Room
		08:00
		09:00
		09:45
Coffee Break		10:30
Session 3 **T3 - OPTIMISATION AND OPTIMAL PROCESS CONTROL AND OPERATION**	**Session 4** **T5 - PROCESS INTEGRATION AND SUSTAINABLE DEVELOPMENT**	
Salon B	***Salon C***	Room
Luis Puigjaner, Metin Türkay	*Jiří Klemeš, Jozef Markoš*	Co-chairmen
T3-412 - An Automated Algorithm for Throughput Maximization Under Fixed Time Horizon in Multipurpose Batch Plants: S-Graph Approach, *Tibor Holczinger, Thokozani Majozi, Mate Hegyhati, Ferenc Friedler*	T5-1 - Topological Impact of Regeneration Unit Constraints upon Water and Wastewater Network, Petrica Iancu, Valentin Pleşu, Vasile Lavric	10:50
T3-131 - Scheduling Challenges in Biopharmaceutical Manufacturing, *Alexandros Koulouris, Charles A. Siletti, Demetri P. Petrides*	T5-116 - An MINLP Reconstruction of Networks for the Collection, Recycling, Treatment and Disposal of Municipal Solid Waste, *Nataša Iršič Bedenik, Zdravko Kravanja*	11:10
T3-441 - Periodic Scheduling of Multiproduct Continuous Plants Using a Multiple Time Grid Continuous-time Formulation, *Pedro M. Castro, Augusto Q. Novais*	T5-163 - General Framework for Solving the Design and Operation of Wastewater Treatment Networks, *Cristina Martín-Sistac, Gerard Escudero, Moisès Graells*	11:30
T3-452 - An Efficient Global Event-Based Continuous-Time Formulation for the Short-Term Scheduling of Multipurpose Batch Plants, *Diego M. Giménez, Gabriela P. Henning*	T5-248 - A Two-stage Approach for the Design of Biomass Conversion Processes, *Rafael Batres, Teppei Nagatomi, Ricardo Martins, Eric Fraga, Yuji Naka*	11:50
T3-505 - A Precedence-based Monolithic Approach to Lot-sizing and Scheduling of Multiproduct Batch Plants, *Carlos Alberto Méndez, Jaime Cerdá*	T5-400 - Comparison of Reverse Flow and Counter-Current Reactors in Case of Selective Catalytic Reduction of Nox, *Claudiu C. Botar-Jid, Paul Ş. Agachi, Davide Fissore*	12:10
Lunch Champions/Cupola Restaurants		12:30

WEDNESDAY, May 30, 2007

Room ***Salon D***

14:00 **POSTER SESSION**

	Session 5 **T1 - MODELLING IN CAPE - NEW HORIZONS**	**Session 6** **T1 - MODELLING IN CAPE - NEW HORIZONS**
Room	***CONSTANTA***	***Salon A***
Co-chairmen	*Mordechai Shacham, Antonis Kokossis*	*Ernesto Martinez, Gintaras Reklaitis*
15:00	T1-474 - Multi-agent Framework for Fault Detection & Diagnosis in Transient Operations *Ng Yew Seng, Rajagopalan Srinivasan*	T1-515 - A Hybrid Optimization Approach to Parameter Estimation, *Richard Faber, Harvey Arellano-Garcia, Günter Wozny*
15:20	T1-429 - Exploring and Improving Clustering based Strategies for Chemical Process Supervision, *Rodolfo V. Tona, Antonio Espuña, Luis Puigjaner*	T1-551 - A Graph-Theory-Base Approach to the Analysis of Large-Scale Plants, *Heinz A Preisig*
15:40	T1-99 - Merging Functional and Conceptual Ontologies, *Manuel Rodríguez*	T1-553 - First Principle Modeling of an Industrial Fluid Catalytic Cracking – the Adaptation of the Model, *Roman Raluca, Zoltán K. Nagy, Paul Ş. Agachi*
16:00	Coffee Break	

Room ***CONSTANTA***

16:20	Awards (Oral / Poster)
16:40	CAPE Special Lecture, Peter Glavič
17:20	ESCAPE17 Closing Session

WEDNESDAY, May 30, 2007

Salon D	Room
POSTER SESSION	14:00

Session 7 **T5 - PROCESS INTEGRATION AND SUSTAINABLE DEVELOPMENT**	**Session 8** **T1 - MODELLING IN CAPE - NEW HORIZONS**	
Salon B	***Salon C***	Room
Gabriela Henning, Walter Wutkovits	*Heinz Preisig, Paul Ş. Agachi*	Co-chairmen
T5-279 - Process Plant Risk Analysis and Modelling, *Jelenka Savkovic-Stevanovic*	T1-584 - Thermodynamic Calculations for Chemical Engineering Using a Simulated Annealing Optimization Method, *Adrian Bonilla-Petriciolet, Juan Gabriel Segovia-Hernández, Florianne Castillo-Borja, Ulisses Ivan Bravo-Sánchez*	15:00
T5-427 - Environmental Impact Assessment of the Vegetable Cultivations using the Pimentel-Euleistein Model. Case Study Arges Lower Watershed, *Cristian Ioja, Maria Pătroescu, Marius Matache, Gabriela Pavelescu, Radu Damian*	T1-605 - Mining of Graphics for Identification of Mechanisms and Trends of Processes, *Yuri Avramenko, Andrzej Kraslawski*	15:20
T5-439 - Simultaneous Fault Diagnosis in Chemical Plants using Support Vector Machines, *Ignacio Yélamos, Gerard Escudero, Moisès Graells, Luis Puigjaner*	T1-362 – Dynamics of Reactive Distillation Processes with Potential Liquid Phase Splitting, *Jignesh Gangadwala, Gabriel Rădulescu, Nicolae Paraschiv, Achim Kienle, Kai Sundmacher*	15:40
Coffee Break		16:00

CONSTANTA	Room
Awards (Oral / Poster)	16:20
CAPE Special Lecture, Peter Glavič	16:40
ESCAPE17 Closing Session	17:20

POSTER PROGRAM, Tuesday, May 29, 2007, Salon D

14:00-15:00

T1S1 Multi-scale modelling – from molecular to whole sites

T1-267 - Neural Network Based Predictions for the Liquid Crystal Properties of Organic Compounds,
Catalin Lisa, Silvia Curteanu

T1S2 System Identification

T1-561 - On-line Neural Network Estimator of Polymerization Plant,
Piyanuch Thitiyasook, Paisan Kittisupakorn and Kwantip Konakom

T1-608 - Nonlinear Observer for Copolymerization Processes,
Christel Rimlinger-Thomann, Nida Sheibat-Othman, Hassan Hammouri

T1S3 Applied Numerical Methods

T1-440 - Modified Bounded Newton Homotopy Method in Solving Sidestream Column Configurations,
Ilkka Malinen, Juha Tanskanen

T1-95 - On a New Family of Sectional Methods for the Solution of the Coagulation Population Balance,
Margaritis Kostoglou, Michael C. Georgiadis

T1S4 CFD and innovative equipment design

T1-162 - Multiscale CFD Simulation of a Methane Steam Reformer for Optimization of the Spatial Catalyst Distribution,
Matthias Pfafferodt, Peter Heidebrecht, Kai Sundmacher, Uwe Würtenberger, Marc Bednar

T1-442 - Modelling heat transfer and fluid flow inside a pressure cooker,
Denis Flick, Richard Rocca, Christophe Doursat, Jean Vasseur

T1-461 - Mixing Computer Algebra and Numerical Methods when Solving CAPE Models,
Karim Alloula, Jean-Pierre Belaud, Jean-Marc LeLann

T1-524 - Detailed investigations of two-liquid phase flows on a packing surface,
Steve Paschke, Ilja Ausner, Yuan Xu, Jens-Uwe Repke, Günter Wozny

T1-643 - Optimising design of secondary combustion chambers using CFD,
Pavel Petr, Ladislav Bebar, Jiri Hajek, Marek Sarlej and Petr Stehlik

T1-644 - Low-NOx burner design evaluation by CFD,
Marek Šarlej, Pavel Petr, and Petr Stehlík

T2S1 From product properties to molecular design

T2-326 - An Algebraic Property Clustering Technique for Molecular Design,
Fadwa T. Eljack, Charles C. Solvason, Mario R. Eden

T2-343 - Simultaneous Polymer Property Modeling using Grid Technology for Structured Products,
Kavitha Chelakara Satyanarayana, Jens Abildskov, Rafiqul Gani

T2-504 - On-Line Monitoring of Particle Shape and Size Distribution in Crystallization Processes through Image Analysis,
Ying Zhou, Xuan-Tien Doan, Rajagopalan Srinivasan

T2-540 - Prediction of Binary Interaction Coefficient and Critical Parameters of Cholesterol in Supercritical Carbon Dioxide,
Hatem Ksibi, Ali Ben Moussa

T2S2 Nanoscale processes and materials

T2-389 - Modelling and Parameter Estimation for Transport Processes in Zeolite Membranes,
Raluca Isopescu, José Sanchez, Cristiana Luminița Gîjiu, Romulus Dima, Ovidiu Muntean

T2-527 - Improving the Efficiency of Membrane Bioreactors by a Novel Model-based Control of Membrane Filtration,
Anja Drews, Harvey Arellano-Garcia, Jan Schöneberger, Jana Schaller, Matthias Kraume, Günter Wozny

T2S3 New or improved process synthesis design

T2-133 - Logic Based Algorithms for the Rigorous Design of Thermally Coupled Distillation Sequences,
José A. Caballero, Ignacio E. Grossmann

T2-188 - Modelling, Design and Optimisation of a Hybrid PSA-Membrane Gas Separation Process,
Charles O. Akinlabi, Dimitrios I. Gerogiorgis, Michael Georgiadis, Efstratios N. Pistikopoulos

T2-214 - Process and Plant Improvement Using Extended Exergy Analysis, a Case Study,
Alhassan S.Tijani, Werner Witt, Ludwig Dietzsch

T2-241 - Design of Non-isothermal Process Water Networks,
Miloš Bogataj, Miguel J. Bagajewicz

T2-28 - Grassroot design of storageless batch plants,
Thomas Pattinson, Thokozani Majozi,

T2-3 - Solvent Selection Evaluation Tools for an Early Stage at Pharmaceutical Process,
Samuel Perez, Paul Sharratt

T2-369 - Axial Dispersion Modeling of Laminar Flames,
Elena Daniela Lavric, Alexander Konnov, Jacques De Ruyck, Vasile Lavric

T2-518 - An Iterative Solution Approach to Process Plant Layout using Mixed Integer Optimisation,
Gang Xu, Lazaros G. Papageorgiou

T2-534 - Nonlinear Behaviour of Reactor-Separator and Reactor-Distillation Networks: Influence of the Energy Balance Formulation,
Klaus-Peter Zeyer, Amol A. Kulkarni, Achim Kienle, Vasudeva Kumar Mantravadi, Pushpavanam Subramanian

T2-89 - Process Synthesis for the Sugar Sector – Computer Based Insights in Industrial Development,
Laszlo Halasz, Gernot Gwehenberger, Michael Nafrodoslawsky

T2-9 - Integrated Knowledge Based System for Process Synthesis,
Abdullah Alqahtani, Klaus Hellgardt, Richard Holdich, Iain Cumming

T3S1 Planning, scheduling and distributed control systems

T3-134 - A Novel Continuous-time MILP Approach for Short-term Scheduling of Multipurpose Pipeless Batch Plants,
Sergio Ferrer-Nadal, Carlos A. Mendez, Moisès Graells, Luis Puigjaner

T3-136 - An Efficient Model Implementation to Solve a Real-world Cutting Stock Problem for a Corrugated Board Boxes Mill,
María Analía Rodríguez, Aldo Vecchietti

T3-176 - Production Scheduling of a Large-Scale Industrial Continuous Plant: Short-Term and Medium-Term Scheduling,
Munawar A. Shaik, Christodoulos A. Floudas, Josef Kallrath, Hans-Joachim Pitz

T3-353 - MISPT: a User Friendly MILP Mixed-time based Production Planning Tool,
Mattias Hästbacka, Joakim Westerlund, Tapio Westerlund

T3-360 - Exploiting the Use of a Flexible Recipe Framework to Manage Financial Risk,
Gonzalo Guillén-Gosálbez, Sergio Ferrer-Nadal, Luis Puigjaner

T3-377 - Multiobjective Optimization Applied to the Distribution of Petroleum Products in Pipelines Networks,
Henrique Westphal, Lúcia Valéria Ramos de Arruda

T3-459 - Rescheduling of Medium Term Pipeline Operation with Tank Farm Inventory Management,
Susana Relvas, Ana Paula Barbosa-Póvoa, Henrique A. Matos, João Fialho

T3-499 - Optimal Planning of Closed Loop Supply Chains: A Discrete versus a Continuous-time formulation,
Ana Cristina Santos Amaro, Ana Paula D. F. Barbosa-Póvoa

T3-514 - A Discrete/Continuous-Time MILP Model For Medium-Term Planning of Single Stage Multiproduct Plants,
Jose M. Pinto, Peter Chen, Lazaros G. Papageorgiou

T3-53 - Learning to schedule new orders in batch plants using aproximate dynamic programming
Facundo Arredondo, Ernesto Martínez

T3-616 - Simulating the Operational Scheduling of a Real-World Pipeline Network,
Fernando Maruyama Mori, Ricardo Lüders, Lúcia Valéria Ramos de Arruda, Lia Yamamoto, Mário Vicente Bonacin, Helton Luis Polli, Mariza Correia Aires, Luiz Fernando de Jesus Bernardo

T3-618 - An Efficient Approach to the Operational Scheduling of a Real-World Pipeline Network,
Flávio Neves-Jr, Leandro Magatão, Sérgio Leandro Stebel, Suelen Neves Boschetto, Luiz Carlos Felizari, Daniel Irineu Czaikowski, Roger Rocha, Paulo César Ribas

T3-636 - Assessment of Discrete Event Simulation Software for Enterprise-wide Stochastic Decision Problems,
Juan Camilo Zapata, Pradeep Suresh, Gintaras V. Reklaitis

T3S3 Hierarchical and optimal process control

T3-138 - Optimal Fed-Batch Bioprocess Control. An Advanced Approach,
Mihai Caramihai, Ana Chirvase, Christian Fonteix, Ivan Marc, Franz Fournier, Raluca Misleanu, Camelia Ungureanu

T3-14 - Design and control analysis of thermally coupled configurations for quaternary distillations
Juan Gabriel Segovia – Hernández, Jesús Rafael Alcántara –Ávila, Julián Cabrera – Ruiz, Salvador Hernández, Ben - Guang Rong

T3-178 - Closed-loop Implementation of Optimal Trajectories in Batch Distillation,
José Espinosa, Jacinto L. Marchetti

T3-185 - Advanced Control of a Reactive Distillation Column,
Zoltan K. Nagy, Reinhardt Klein, Anton A. Kiss, Rolf Findeisen

T3-340 - Nonlinear Predictive Control of a pH Process,
Corneliu Lazăr, Răzvan Pintea, Robin De Keyser

T3-446 - Control System Pcs7 and M.I.S. Together for the Complete Automation of the Process in the Sugar Beet Factory of Co.Pro.B. – Minerbio – Italy,
Sandro Castaldini

T3-486 - Five Formulations of Extended Kalman Filter: Which is the best for D-RTO?,
Nina Paula Gonçalves Salau, Argimiro Resende Secchi, Jorge Otávio Trierwieler

T3-570 - A Tool for Kalman Filter Tuning,
Bernt M. Åkesson, John Bagterp Jørgensen, Niels Kjølstad Poulsen, Sten Bay Jørgensen

T4S1 Bioproducts and biomaterials

T4-230 - Bioethanol Production Sustainability: Outlook for Improvement using Computer-Aided Techniques,
Elmer Ccopa Rivera, Aline Carvalho da Costa, Rubens Maciel Filho

T4-244 - Modeling of Counter Current Monoclonal Antibody Extraction using Aqueous Two-Phase Systems,
Joachim Ahmed Samatou, Annebart Engbert Wentink, Paula Alexandra J. Rosa, Ana Margarida Azevedo, Maria Raquel Aires-Barros, Werner Bäcker, Andrzej Górak

T4-356 - A by-product oriented simulator with structured model: application for acrylic acid production from renewable sources,
Betânia H. Lunelli, Rubens Maciel Filho, Maria R. W. Maciel, Eduardo C. Vasco de Toledo, Dile P. Stremel

T4-379 - Strain improvement and mediator selection for microbial fuel cell by genome scale in silico model,
Rajib Saha, Selvarasu Suresh, Wonjun Park, Dong-Yup Lee, Iftekhar A. Karimi

T4-458 - CFD Simulation of concentration profiles and velocity field. Application: in bioleaching process,
Mohammad Mousavi, Arezou Jafari, Soheila Yaghmaei, Manouchehr Vossoughi, Ilkka Turunen, Mohammad Reza Kamali, Pertti Sarkomaa

T4-511 - A CAPE Approach to gamma-Linolenic Acid Production via Lipase-Cata-lyzed Enzymatic Hydrolysis,
Patricia B. Lucente Fregolente, Elmer C. Rivera, Leonardo Vasconcelos Fregolente, Patricia de Oliveira Carvalho, Aline Costa, Maria Regina Wolf-Maciel, Rubens Maciel Filho

T4-52 - Parameter Identification for a Mechanistic Model of Poly-β-hydroxy-butyrate Production,
Mark A. Pinto, Charles D. Immanuel

T4-625 - Research regarding obtaining volatile oils from native plants in microwave assisted vacuum systems,
Moşteanu Daniel, Miclăuş Simona, Bârsan Ghiță

T5S1 Process intensification

T5-146 - Systematic retrofit design of batch processes using an indicator and model based framework,
Levente L. Simon, Ulrich Fischer, Konrad Hungerbühler

T5-252 - A Design Method for Internal Heat Integrated Distillation Columns (iHIDiCs),
Mamdouh Gadalla, Zarko Olujic, Laureano Jiménez Esteller, Gonzalo Guillén-Gosálbez

T5-270 - Optimal Operation of the Cyclic Claus Process,
Assanousi Abufares, Sebastian Engel

T5-57 - Minimum Reflux in Liquid–Liquid Extraction,
Santanu Bandyopadhyay, Calin-Cristian Cormos

T5-613 - Recovery of Aromatics from Pyrolysis Gasoline by Conventional and Energy-Integrated Extractive Distillation,
Faten Abushwireb, Hadi Elakrami, Mansour Emtir

T5S2 Combined heat and power site-level integration

T5-135 - Steam CHPP Site Level Optimal Integration into a Refinery/Petrochemical Plant,
Victor Eduard Cenuşă, Horia Ionuț Petcu, Florin Niculae Alexe

T5-201 - Integrating Recovered Jetty Boil-off Gas as a Fuel in an LNG Plant,
Danan S. Wicaksono, Iftekhar A. Karimi, Hassan Alfadala, Omar I. Al-Hatou

T5-255 - Modelling, Investment Planning and Optimisation for the Design of a Polygeneration Energy System,
Pei Liu, Dimitrios I. Gerogiorgis, Efstratios N. Pistikopoulos, Diogo Narciso

T5-44 - Steam System Design Using a Novel Graphical Targeting Method and MILP Model,
Sternberg Willem Andries Coetzee, Thokozani Majozi

T5-473 - Review of Optimization Models for the Design of Polygeneration Systems in District Heating and Cooling Networks,
Jordi Ortiga, Joan Carles Bruno, Alberto Coronas, Ignacio E. Grossmann

T5-606 - Design and Optimization of District Energy Systems,
Céline Weber, François Maréchal, Daniel Favrat

T5S3 Life cycle modelling

T5-105 - Adaptive Control Approach in Modeling Life-cycle Maintenance Policy Selection and Optimisation During Infrastructure Systems Conceptual Design & Operation,
Augustine N. Ajah, Johan Grievink, Paulien Herder, Margot Weijnen

T5-247 - A Web-based Infrastructure for Integrated Life-cycle Engineering,
Rafael Batres, Kazumasa Hayashi, Yoshiaki Shimizu

T5-579 - Small Scale and Large Scale Plants – Effect on Life Cycle Assessment,
Maiya Shibasaki, Stefan Albrecht , Thilo Kupfer, Michael Held

T5-59 - Extension of Computer-Aided Process Engineering Applications to Environmental Life Cycle Assessment and Supply Chain Management,
William M. Barrett, Svetlana Strunjaš-Yoshikawa, Jonathan H Bell

T5-607 - Modeling of Main Material and Energy Flows of a Chemicals Company and LCA of Products thereof,
Christiane Richard-Elsner, Christiane Glasmacher-Remberg

T5S5 Bio diesel and sustainable fuels

T5-316 - Ethanol From Lignocellulosic Biomass: A Comparison Between Conversion Technologies,
Chiara Piccolo, Fabrizio Bezzo

T5-86 - Process for Fatty Acid Methyl Esters by Dual Reactive Distillation,
Alexandre C. Dimian, Florin Omota, Anton A. Kiss

POSTER PROGRAM, Wednesday, May 30, 2007, Salon D

14:00-15:00

T1S6 Improving modelling & simulation

T1-107 - Modelling and Simulation of Multi-bed Pressure Swing Adsorption Processes,
Dragan Nikolic, Apostolos Giovanoglou, Michael C. Georgiadis, Eustathios S. Kikkinides

T1-190 - Experience on Gridification and Hyper-infrastructure Experiments in Optimization and Process Synthesis,
Du Du, Siyu Yang, Antonis C. Kokossis, Patrick Linke

T1-249 - Flexibility Study on Site-Modeling,
Kentaro Hirata, Pang Chan, Haruo Sakamoto, Chi-Wai Hui, Sau-Man Lai

T1-312 - Measurement of Plant Flexibility,
Sau-Man Lai, Chi-Wai Hui

T1-313 - Computer Aided Operation and Design of the Cationic Surfactants Production,
Jelenka Savkovic-Stevanovic, Tatjana Mošorinac, Snežana B.Krstic, Ružica D.Beric

T1-318 - A computer based platform to model the intrinsic and final properties of PEAD: application for the injection plastic molding
Maria Carolina B. Costa, André L. Jardini, Marcelo Embiruçu, Maria Regina Wolf Maciel, Rubens Maciel Filho

T1-320 - Recycled Liquid Membranes Use for Oxalic Acid Recovery. Mathematical Model and Functional Optimization,
Daniel Dinculescu, Vasile Lavric

T1-347 - Computer-Aided Multiscale Modelling for Chemical Process Engineering,
Ricardo Morales-Rodríguez, Rafiqul Gani

T1-381 - Modeling and Simulation of Main Cryogenic Heat Exchanger in a Base-load Liquefied Natural Gas Plant,
M M Faruque Hasan, Iftekhar A Karimi, Hassan Alfadala, Henk Grootjans

T1-406 - Modelling reactive separations with very fast chemical reactions,
Juraj Sláva, Jozef Markoš

T1-416 - Optimal Location of Booster Disinfection Stations in a Water Distribution System: A Two-Stage Stochastic Approach,
Vicente Rico-Ramirez, Francisco Gomez-De la Cruz, Gustavo Iglesias-Silva, Salvador Hernandez-Castro

T1S7 Artificial Intelligence

T1-141 - Computer aided quality management for a wide class of phosphorus containing products based on information CALS-technologies,
Arkadiy Bessarabov, Eugeny Y. Kenig, Tatyana Ogorodnikova, Olga Zhdanovich

T1-183 - Adaptive Controller Tunning by Kalman Filter for Advanced application to a Fermentation Process,
Elis R. Duarte, Laércio Ender, Daniel I. P. Atala, Rubens Maciel Filho

T1-332 - Code Design as an Optimization Problem: from Mixed Integer Programming to an Improved High Performance *Randomized* GRASP like Algorithm,
José Barahona da Fonseca

T1-415 - Mathematical Model and control for Gas Phase Olefin Polymerization in Fluidized-Bed Catalytic Reactors,
Ahmmed Saddi Ibrehem, Mohamed Azlan Hussain, Nayef Mohamed Ghasem

T1-430 - Opportunities for Agent-Based Models in Computer Aided Process Engineering,
Koen H. van Dam, Zofia Lukszo, Rajagopalan Srinivasan, Iftekhar A. Karimi

T1-516 - A Mixed Integer Optimisation Approach for Data Classification with Multiple Groups,
Gang Xu, Nan Shao, Lazaros G. Papageorgiou

T1-8 - Neural and Genetic based Techniques for Solving the MSF Model as Opposed to Conventional Numerical Methods,
Farouq Mjalli, Nabil Abdel-Jabbar, Hazim Qiblawey, Hisham Ettouney

T2S4 Integrated process and product design

T2-269 - An umbrella-like approach for design of crystals with specified properties,
Caliane Bastos Borba Costa, Rubens Maciel Filho

T2-335 - Workflow Challenges During Front-End Engineering,
Arvind G. N. Patel

T2-445 - Design and Scheduling of Periodic Multipurpose Batch Plants under Uncertainty,
Tânia Rute Pinto, Ana Paula F. D. Barbósa-Póvoa, Augusto Q. Novais

T2-49 - Integration of Process Modeling with Laboratory Experiments in Conceptual Design: Bio-based Glycerol Dehydration Case Study,
Jeffrey R. Seay, Mario R. Eden, Robert D'Alessandro, Thomas Thomas, Hubert Redlingshoefer, Christoph Weckbecker, Klaus Huthmacher

T2-61 - OptWatNet - A Software for the Optimal Design of Water-Using Networks with Multi-contaminants,
João P. Teles, Pedro M. Castro, Augusto Q. Novais

T2S5 CAPE for Oil & Gas Processes

T2-192 - CFD Study of Gas Mixing Efficiency and Comparisons with Experimental Data,
Edward Rój, Marek Dmoch

T2-358 - Modeling of Trickle Bed Reactor for Hydrotreating of Vacuum Gas Oils: Effect of Kinetic Type on Reactor Modeling,
Favio Jiménez, Karina Ojeda, Eduardo Sánchez, Viatcheslav Kafarov, Rubens Maciel Filho

T2-380 - Olexan: A Tool for Online Exergy Analysis,
Maryam Zargarzadeh, Iftekhar A. Karimi, Hassan Alfadala

T2-391 - Modeling and Simulation of Organic Compounds Adsorption Process in Brazilian Oil Shale,
Rosalvo Stachiw, Flavio Neves Júnior, Lúcia Valéria Ramos de Arruda, Livia Mari Assis

T2-517 - An Efficient Approach to Robust Simulation of Claus Processes in Coking Plants,
Jan Schöneberger, Harvey Arellano-Garcia, Holgert Thielert, Günter Wozny

T2-591 - Model Requirement for Control Design of an LNG Process,
Arjun Singh, Morten Hovd

T2S6 CAPE – industrial success stories

T2-200 - Making soda ash manufacture more sustainable. A modeling study using ASPEN Plus,
Ana-Maria Cormoş, Călin-Cristian Cormoş, Paul Ş. Agachi

T2-345 - Optimization of the equipment positioning in manufacture of Tissue Paper,
Daniela M.Devienne Drummond, Reginaldo Guirardello

T2-357 - Weighted Residuals Method Applied to the Filament Winding Process,
Rogério Luz Pagano, Evaristo Chalbaud Biscaia Jr, Verônica Calado

T2-457 - Modelling and Optimisation of a Rinsing Process in a Recycled Plastic Plant,
Piyanuch Thitiyasook, Paisan Kittisupakorn, Sathit Niamsuwan, Kwantip Konakom

T3S2 System diagnosis and management of supply chain

T3-159 - Design of recovery supply chains: a Portuguese recovery network for WEEE,
Maria Isabel Gomes Salema, Ana Paula Barbosa-Póvoa, Augusto Q. Novais, Mónica Luizio

T3-229 - A Performance Assessment Framework for Supply Chain Networks,
Sundar Raj Thangavelu, Lakshminarayanan Samavedham

T3-232 - A Joint Control Framework for Supply Chain Planning,
José Miguel Laínez, Antonio Espuña, Luis Puigjaner

T3-245 - Combined Use of Model based Data Validation and Data Driven Techniques for Process Monitoring,
Arnaud Duchesne, Georges Heyen, Philippe Mack, Boris Kalitventzeff

T3-246 - Logistics Optimization Using Hybrid Meta-heuristic Approach under Very Realistic Conditions,
Yoshiaki Shimizu, Takeshi Wada, Yoshihiro Yamazaki

T3-349 - Genetic Algorithm Optimization of Fractional Crystallization Processes,
Raluca Isopescu, Alexandru Woinaroschy, Laurențiu Filipescu

T3-383 - Outsourcing and Optimization of Logistics Services for Chemical Companies,
Mukta Bansal, Iftekhar A. Karimi, Rajagopalan Srinivasan

T3-404 - Constraint Programming based Multi-objective Sensor Network Design for Fault Diagnosis,
Prakash R. Kotecha, Mani Bhushan, Ravindra D. Gudi

T3-414 - Analysis of the Runaway in an Industrial Heterocatalytic Reactor,
Tamás Varga, Ferenc Szeifert, József Réti, János Abonyi

T3-451 - Industrial Supply Chains: Performance Measures, Metrics and Benchmarks,
Alicia C. Böhm, Horacio P. Leone, Gabriela P. Henning

T3-595 - Identifying Added Value in Integrated Oil Supply Chain Companies – a Case Study,
Zaid Laftah, Tengku Zeti Tengku Abdul Aziz, I.D.L. Bogle

T3-642 - Multi-Objective Optimization of Dairy Supply Chain,
Natasha Vaklieva-Bancheva, Antonio Espuña, Elisaveta Shopova, Luis Puigjaner, Boyan Ivanov

T3S4 Control-oriented integrated design

T3-137 - Pareto optimal design and operation of multivessel batch distillation,
Sven Gruetzmann, Matthias Leipold, Georg Fieg

T3-157 - Comprehensive Process Investigation Methodology for Energy-Integrated Distillation,
Hajnalka Kencse, Peter Mizsey

T3-22 - Design and Control of Thermally Coupled and Heat Integrated Distillation Sequences for Quaternary Separations,
Jorge Alberto Porras-Rodríguez, Héctor Hernández-Escoto, Juan Gabriel Segovia-Hernández, Salvador Hernández

T3-224 - Process Modeling and Simulation for Optimization of Operating Processes,
Balazs Balasko, Sandor Nemeth, Akos Janecska, Tibor Nagy, Gabor Nagy, Janos Abony

T3-407 - Improved Analytical PID Controller Design for the Second Order Unstable Process with Time Delay,
M. Shamsuzzoha, Jongpal Jeon, Moonyong Lee

T3-431 - Dynamic Simulation and Analysis of a Solid Oxide Fuel Cell (SOFC),
Debangsu Bhattacharyya, Raghunathan Rengaswamy, Caine Finnerty

T3-475 - Study of an Integrated System for the Production of Hydrogen by Autothermal Reforming of Methanol,
Dimitrios Ipsakis, Panagiotis Kechagiopoulos, Christina Martavaltzi, Spyridon Voutetakis, Panos Seferlis, Prodromos Daoutidis, Fotis Stergiopoulos

T3-94 - Iterative Specification Refinement in Deriving Logic Controllers,
Sven Lohmann, Lan Anh Dinh Thi, Thanh Ha Tran, Olaf Stursberg, Sebastian Engell

T4S3 Systems biology and modelling of metabolic processes

T4-123 - Automatic Synthesis of Alternative Paths of Biochemical Networks using Model Checking,
Jinkyung Kim, Il Moon

T4-164 - A Novel Clustering Approach: Global Optimum Search with Enhanced Positioning,
Meng P. Tan, James R. Broach, Christodoulos A. Floudas

T4-204 - Mathematical Modeling of Single Cell Protein and Ethanol Production by *Kluyveromyces cicerisporus* Fermentation on Whey,
Márcia Peixoto Vega, Rodrigo da Silva Leite, Maria Alice Cruz Lopes de Oliveira

T4-395 - Evaluation of sunflower collection by genetic variability based on germination and plantlet development parameters using Artificial Neural Networks,
Dorina Bratfalean, Mircea Vasile Cristea, Paul Ş. Agachi, Dan Florin Irimie, Ahmad Sarrafi, Michel Petitprez

T4-498 - A PCA-Based Approach for Gene Target Selection to Improve Industrial Strains,
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T5S4 Safety analysis, risk assessment, and environmental impact

T5-101 - A Hierarchical Approach for the Estimation of Environmental Impact of a Chemical Process: from Molecular Modeling to Process Simulation,
Maurizio Fermeglia, Gennaro Longo, Letitia Toma

T5-219 - Integrated Design of Process and Operation Considering Local Risks and Globalimpacts: A Case Study on Metal-degreasing Process Design
Yasunori Kikuchi, Masahiko Hirao

T5-409 - Safety analysis of a heterogeneous catalytic tubular reactor for complex reactions,
Pavol Laššák, Jozef Markoš, Ľudovít Jelemenský

T5-410 - Impact of Mathematical Model Selection on Prediction of Steady State and Dynamic Behaviour of a Reactive Distillation Column,
Zuzana Švandová, Juraj Labovský, Jozef Markoš, Ľudovít Jelemenský

T5-418 - Design, Optimization and Safety Analysis of a Heterogeneous Tubular Reactor by using the HAZOP Methodology,
Juraj Labovský, Pavol Laššák, Jozef Markoš, Ľudovít Jelemenský

T5-449 - Combining Disturbance Simulation and Safety Analysis Techniques for Improvement of Process Safety and Reliability,
Naveed Ramzan, Werner Witt

T5-547 - Global modelling with LIS for water pollution,
Costica Nitu , Anda Sabena Dobrescu

T5-145 - Risk of Gaseous Release Assessment Based on Artificial Intelligence Methods,
Călin Ioan Anghel, Alexandru Ozunu

T5-98 - Functional Modeling for Risk Analysis,
Manuel Rodríguez, José Luis de la Mata

T5S6 Waste management

T5-29 - Towards an effective scheduling technique for zero-effluent multipurpose batch plants,
Jacques F. Gouws, Thokozani Majozi

T5-450 - Artificial Neural Networks Based Model Predictive Control of the Wastewater Treatment Plant,
Mircea V. Cristea, Paul Ş. Agachi

T5-490 - State Detection of a Wastewater Treatment Plant,
Aki Sorsa, Kauko Leiviskä

T5-55 - Process Water Management with Regeneration and Recycle,
Călin-Cristian Cormoş, Santanu Bandyopadhyay

T5-609 - Targeting the Freshwater for Water Networks with Single Contaminant,
Zhi-Yong Liu, Yu-Zhen Yang, Yan-Mei Li

T5-645 - Novel types of equipment for off-gas cleaning,
Radek Dvorak, Vitezslav Masa, Petr Chlapek, Kirill Solodyankin

T5-646 - Emissions abatement in Waste-to-Energy Systems,
Tomas Parizek, Ladislav Bebar, Jaroslav Oral, Petr Stehlik