



**ESCAPE-16**  
+  
**PSE'2006**

**July 9 – 14, 2006**  
**Garmisch-Partenkirchen**  
**Germany**

**Sunday, July 9, 2006**

- 10:00 – EFCE Working Party on Computer Aided Process Engineering (CAPE-WP)
- 12:00
- 13:30 – Business Meeting of the CAPE-WP
- 16:30
- 16:00 Registration
- 18:00 Welcome Reception in the Foyer of the Congress Center
- 20:00 World Championship Soccer Final  
Live TV Coverage on Large Screen at the Congress Center

Monday, July 10, 2006

Program PSE/ESCAPE 2006

Room *Festsaal Werdenfels*

09:00 – **Opening Remarks**  
09:20 - DECHEMA  
- EFCE & CAPE Working Party  
- IPC Chairmen

09:25 - **PhD Award Ceremony**  
09:45

9:45 - **Plenary Lecture**  
10:30 **Innovation in the chemical industry: a growth engine!**  
S. Marcinowski, BASF Aktiengesellschaft, Ludwigshafen/D

10:30 *Coffee Break*

Topic	Modelling and Numerical Methods	Product and Process Design	Operations and Control	Business Decision Support
Room	<i>Festsaal Werdenfels</i>	<i>Konzertsaal Richard Strauss</i>	<i>Olympiasaal</i>	<i>Zugspitze I+II</i>
10:45	<b>Stochastic grey-box modeling of the enzymatic biochemical reaction network of <i>E. coli</i> mutants</b> <u>F. Davidescu</u> , H. Madsen, Technical University of Denmark, Lyngby/DK; M. Schümperli, M. Heinemann, S. Panke, ETH Zürich/CH; S.B. Jørgensen, Technical University of Denmark, Lyngby/DK	<b>Integrated approach to crystallization process design for fine chemicals and pharmaceuticals</b> <u>C. Wibowo</u> , K.D. Samant, L. O'Young, ClearWaterBay Technology Inc., Walnut, CA/USA	10:45 <b>Differential recurrent neural network based predictive control</b> R. Al Seyab, <u>Y. Cao</u> , Cranfield University, Bedford/UK	<b>Dynamic rule-based genetic algorithm for large-size single-stage batch scheduling</b> <u>Y. He</u> , C.W. Hui, Hong Kong University of Science and Technology/PRC
11:10	<b>OPEN CHEMASIM™: breaking paradigms in process simulation</b> <u>H. Hasse</u> , University of Stuttgart/D; B. Bessling, R. Böttcher, BASF Aktiengesellschaft, Ludwigshafen/D	<b>Real-time imaging and product quality characterization for control of particulate processes</b> <u>Y. Zhou</u> , Institute of Chemical and Engineering Sciences and National University of Singapore/SGP; X.T. Doan, Institute of Chemical and Engineering Sciences, Singapore/SGP; R. Srinivasan, Institute of Chemical and Engineering Sciences and National University of Singapore/SGP	11:10 <b>Coordinator MPC with focus on maximizing throughput</b> <u>E.M.B. Aske</u> , Norwegian University of Science and Technology and Statoil R&D, Trondheim/N; S. Strand, Statoil R&D, Trondheim/N; S. Skogestad, Norwegian University of Science and Technology, Trondheim/N	<b>Slot-based vs. global event-based vs. unit-specific event-based models in scheduling of batch plants</b> M.A. Shaik, S.L. Janak, <u>C.A. Floudas</u> , Princeton University, NJ/USA
11:35	<b>Risk analysis and robust design under technological uncertainty</b> R.F. Blanco-Gutierrez, <u>C.C. Pantelides</u> , C.S. Adjiman, Imperial College London/UK	<b>Multi-objective optimization of fixed-bed ion exchange processes for phytopharmaceutical production</b> C.M. Silva, A.G. Barreto Jr., <u>E.C. Biscaia Jr.</u> , Universidade Federal do Rio de Janeiro/BR	11:35 <b>Systematic methodology for reproducible optimizing batch operation</b> <u>S.B. Jørgensen</u> , D. Bonn�, Technical University of Denmark, Lyngby/DK	<b>Stochastic integer programming in chemical batch scheduling: evolution strategies vs. exact algorithms</b> <u>J. Till</u> , G. Sand, S. Engell, Universit�t Dortmund/D
12:00 - 13:30	<i>Lunch Break</i>			

Room Festsaal Werdenfels

13:30

**Keynote Lecture**  
**Recent developments in the risk management of offshore production systems**

D. Averbuch, Institut Français du Pétrole (IFP), Rueil-Malmaison/F

14:20 -  
14:25 *Time for room change*

**Topic Modelling and Numerical Methods Product and Process Design**

Room Festsaal Werdenfels

14:25

**A performance comparison of some high breakdown robust estimators for nonlinear parameter estimation**

E.L.T. Conceição, A.T.G. Portugal, University of Coimbra/P

**Computer aided methods & tools for separation & purification of fine chemical & pharmaceutical products**

M. Afonso, Instituto Superior Técnico, Lisbon/P; V. Soni, P. Mitkowski, L. d'Anterrosches, R. Gani, Technical University Denmark, Lyngby/DK; H. Matos, Instituto Superior Técnico, Lisbon/P

14:50

**Simultaneous dynamic validation/identification of mechanistic process models and reconciliation of industrial process data**

P.A. Rolandi, Process Systems Enterprise Ltd., London/UK; J.A. Romagnoli, Louisiana State University, Baton Rouge, LA/USA

**Methodology for the design of industrial hydrogen networks and the optimal placement of purification units using multi-objective optimisation techniques**

L. Girardin, F.M.A. Marechal, Ecole Polytechnique Federale de Lausanne/CH; P. Tromeur, Air Liquide, Jouy-en-Josas/F

15:15

**A model discrimination based approach to the determination of operating regimes for chemical reactors**

A. Yang, E.B. Martin, G. Montague, A.J. Morris, University of Newcastle/UK

**Dynamic modelling of complex batch distillation starting from ambient conditions**

S. Grützmann, Hamburg University of Technology/D; T. Kapala, Cognis Deutschland GmbH & Co. KG, Düsseldorf/D; G. Fieg, Hamburg University of Technology/D

15:40 -  
17:20 **Coffee Break & Poster Session 1 – Topics „Product and Process Design“ and „Business Decision Support“**

Konzertsaal Richard Strauss

13:30

**Keynote Lecture**  
**Supply chain design, management and optimization**  
D. Kassmann, R. Allgor, Amazon.com, Seattle, WA/USA

**Infrastructure Systems**

Olympiasaal

14:25

**Energy planning in buildings under uncertainty in fuel costs: the case of a hospital in Greece**

G. Mavrotas, K. Florios, P. Georgiou, National Technical University of Athens/GR

14:50

**Modelling an electricity infrastructure as a multi-agent system - lessons learnt from manufacturing control**

K.H. van Dam, M. Houwing, Z. Verwater-Lukszo, I. Bouwmans, Delft University of Technology/NL

15:15

**Agent-enabled dynamic management system for process plants**

A. Kokossis, University of Surrey, Guildford/UK; Z. Shang, Cranfield University/UK; E. Gao, University of Surrey, Guildford/UK

**Business Decision Support**

Zugspitze I+II

**Routing and cargo allocation planning of a parcel tanker**

K.H. Neo, National University of Singapore/SGP; H.C. Oh, The Logistics Institute - Asia Pacific; L.A. Karimi, National University of Singapore/SGP

**Multi-period capacitated lot sizing with variable batch sizes**

Y.C. See Toh, Imperial College London/UK; S.P.K. Walsh, ICI Paints, Slough/UK; N. Shah, Imperial College London/UK

**A framework for capturing the impact of resource allocation policies in the selection of a new product portfolio**

J.C. Zapata, Purdue University, West Lafayette, IN/USA; V.A. Varma, Air Products and Chemicals, Allentown, PA/USA; G.V. Reklaitis, Purdue University, West Lafayette, IN/USA

Topic	Modelling and Numerical Methods	Product and Process Design	Operations and Control	Business Decision Support
Room	<i>Festsaal Werdenfels</i>	<i>Konzertsaal Richard Strauss</i>	<i>Olympiasaal</i>	<i>Zugspitze I+II</i>
17:25	<b>Optimal experimental design for ill-posed problems</b> A. Bardow, ETH Zürich/CH	<b>Separation of azeotropes in batch extractive stripper with intermediate entrainer</b> V. Varga, BUTE, Budapest/H and ENSIACET, Toulouse/F; E.R. Frits, BUTE and HAS RGTC, Budapest/H; V. Gerbaud, ENSIACET, Toulouse/F; Z. Fonyo, HAS RGTC, Budapest/H; X. Joulia, ENSIACET, Toulouse/F; Z. Lelkes, BUTE, Budapest/H; <u>E. Rev</u> , BUTE and HAS RGTC, Budapest/H	17:25 <b>Hybrid model predictive control of a sugar end section</b> <u>D. Sarabia</u> , C. de Prada, S. Cristea, R. Mazaeda, University of Valladolid/E	<b>A unified approach for knowledge modeling in pharmaceutical product development</b> <u>C. Zhao</u> , A. Jain, L. Hailemariam, G. Joglekar, V. Venkatasubramanian, K. Morris, G. Reklaitis, Purdue University, West Lafayette, IN/USA
17:50	<b>Modelling deammonification in biofilm systems: sensitivity and identifiability analysis as a basis for the design of experiments for parameter estimation</b> <u>D. Brockmann</u> , K.-H. Rosenwinkel, University of Hanover/D; E. Morgenroth, University of Illinois, Urbana-Champaign, IL/USA	<b>Conceptual design of reactive distillation flowsheets</b> <u>G. Daniel</u> , P. Patil, M. Jobson, The University of Manchester/UK	17:50 <b>Control of the synthesis section of a urea plant by means of an MPC controller</b> <u>O.M. Agudelo Manozca</u> , Katholieke Universiteit Leuven/B; J.J. Espinosa Oviedo, IPCOS N.V ISMC, Leuven/B; J. Vandewalle, Katholieke Universiteit Leuven/B	<b>A decision support tool for process optimization of sulphur free diesel production</b> <u>Z. Verwater-Lukszo</u> , M. Salverda, Delft University of Technology/NL; P. Bosman, Shell Nederland Raffinaderij BV, Rotterdam/NL
18:15 - 18:40	<b>A framework for model-based design of parallel experiments in dynamic systems</b> F. Galvanin, M. Barolo, F. Bezzo, Università di Padova/I; <u>S. Macchietto</u> , Università di Padova/I and Imperial College London/UK	<b>Innovative flowschemes using dividing wall columns</b> <u>M.A. Schultz</u> , UOP, Des Plaines, IL/USA; D.E. O'Brien, Jacobs Engineering, Chicago, IL/USA; R.K. Hoehn, C.P. Luebke, D.G. Stewart, UOP, Des Plaines, IL/USA	18:15 - 18:40 <b>Predictive control of polymerization batch reactors using hybrid models</b> <u>J.J. Espinosa Oviedo</u> , W. van Brempt, IPCOS, Leuven/B	<b>Development of a multiobjective scheduler for semiconductor manufacturing</b> O. Baez Senties, <u>C. Azzaro-Pantel</u> , L. Pibouleau, S. Domenech, Laboratoire de Génie Chimique, Toulouse/F
19:00	<i>or 20:00 Public Chamber Orchestra – free of charge (to be confirmed)</i>			

Tuesday, July 11, 2006

Program PSE/ESCAPE 2006

Room Festsaal Werdenfels

8:30 -  
9:20

**Keynote Lecture**

**Life cycle modelling in the chemical industries: is there any reuse of models in automation and control?**

J. Bausa, BASF Aktiengesellschaft, Ludwigshafen/D; G. Dünnebier, Bayer Technology Services GmbH, Leverkusen/D

09:20 –  
09:25

*Time for room change*

**Topic Modelling and Numerical Methods**

Room Festsaal Werdenfels

09:25

**Equivalent dynamic solution of an industrial HDPE slurry reactor**

S. Nigam, K.M. Moudgalya, A.K. Pani, IIT Bombay, Mumbai/IND

09:50

**Stability analysis of differential-algebraic equations in AUTO\_DAE**

B.C. von Clausbruch, E.C. Biscaia, P.A. Melo, Universidade Federal do Rio de Janeiro/BR

10:15

*Coffee Break*

**Topic Modelling and Numerical Methods**

10:45

**Floating index of inequality constrained DAE systems**

D.F.S. Souza, Universidade Federal do Rio de Janeiro/BR; R.C. Vieira, PETROBRAS, Rio de Janeiro/BR; E.C. Biscaia Jr., Universidade Federal do Rio de Janeiro/BR

11:10

**Validated solution of ODEs with parametric uncertainties**

Y. Lin, M.A. Stadtherr, University of Notre Dame, IN/USA

**Topic Product and Process Design**

Room Konzertsaal Richard Strauss

**A computer-aided methodology with robust design criteria for selection of solvents for reactions**

M. Folic, C.S. Adjiman, E.N. Pistikopoulos, Imperial College London/UK

**Systematic procedure for designing a microreactor with slit-type mixing structure**

O. Tonomura, T. Takase, M. Kano, S. Hasebe, Kyoto University/J

**Topic Product and Process Design**

**Scope for process systems engineering studies in Proton Exchange Membrane Fuel Cells (PEMFC): a review of opportunities**

R. Madhusudana Rao, T. Oh, R. Rengaswamy, Clarkson University, Potsdam, NY/USA

**A framework for innovation in process development for heterogeneously catalysed gas-phase reaction systems**

D. Montolio-Rodriguez, University of Surrey, Guildford/UK; D. Linke, Institute for Applied Chemistry Berlin-Adlershof/D; P. Linke, University of Surrey, Guildford/UK

Room Konzertsaal Richard Strauss

8:30 -  
9:20

**Keynote Lecture**

**Challenges for process system engineering in infrastructure operation and control**

Z. Lukszo, M.P.C. Weijnen, R.R. Negenborn, B. De Schutter, Delft University of Technology/NL; M. Ilic, Carnegie Mellon University, Pittsburgh, PA/USA

**Topic Operations and Control**

Room Olympiasaal

09:25 **Model-based optimization for operational policies in seeded cooling crystallization**

A. Abbas, Nanyang Technological University, Singapore/SGP; S.M. Nowee, University of Sydney/AUS; J.A. Romagnoli, Louisiana State University, Baton Rouge, LA/USA

09:50 **Dynamic optimization of molecular weight distribution using orthogonal collocation on finite elements and fixed pivot methods: an experimental and theoretical investigation**

A. Krallis, D. Meimaroglou, V. Saliakas, C. Chatzidoukas, C. Kiparissides, Aristotle University of Thessaloniki/GR

**Topic Infrastructure Systems**

10:45 **Disturbance propagation and rejection models for water allocation network**

X. Feng, R. Shen, Xi'an Jiaotong University/PRC

11:10 **Global optimization of multiscenario mixed integer nonlinear programming models arising in the synthesis of integrated water networks under uncertainty**

R. Karuppiah, I.E. Grossmann, Carnegie Mellon University, Pittsburgh, PA/USA

**Topic Operations and Control**

Room Zugspitze I+II

**Explicit parametric controller for a batch polymerization system**

M. Asteasuain, PLAPIQUI, Bahia Blanca/RA; K. Kouramas, Imperial College London/UK; V. Sakizlis, Bechtel Ltd., London/UK; E.N. Pistikopoulos, Imperial College London/UK

**An approach to linear control of nonlinear processes**

T. Schweickhardt, F. Allgöwer, University of Stuttgart/D

**Topic Business Decision Support**

**Semantic analysis for identification of portfolio of R&D projects - example of microencapsulation**

A. Kraslawski, Lappeenranta University of Technology/FIN

**On the dynamic management of chemical engineering knowledge using an ontology-based approach**

A. Kokossis, E. Gao, A. Kourakis, University of Surrey, Guildford/UK

11:35 **Parameter estimation for stochastic differential equations: algorithm and application to polymer melt rheology**  
B. Pereira Lo, A.J. Haslam, C.S. Adjiman, Imperial College London/UK

**Linking experiments to modeling in biodiesel production**  
A.A. Kiss, A.C. Dimian, G. Rothenberg, University of Amsterdam/NL

11:35 **Hierarchical markov reliability / availability models for energy & industrial infrastructure systems conceptual design**  
A.N. Ajah, P.M. Herder, J. Grievink, M.P.C. Weijnen, Delft University of Technology/NL

**Ontology-based information management in design processes**  
S.C. Brandt, J. Morbach, M. Miatidis, M. Theißen, RWTH Aachen University/D; M. Jarke, RWTH Aachen University/D and Fraunhofer FIT, St. Augustin/D; W. Marquardt, RWTH Aachen University/D

12:00 - 13:30 *Lunch Break*

Room *Festsaal Werdenfels*

13:30 **Keynote Lecture**  
**Challenges and opportunities in process innovation**  
 L.R. Genskow, The Procter and Gamble Company, West Chester, OH/USA

*Konzertsaal Richard Strauss*

13:30 **Keynote Lecture**  
**Recent developments and industrial applications of data-based process monitoring and process control**  
M. Kano, Kyoto University/J; Y. Nakagawa, Sumitomo Metals (Kokura), Ltd., Kitakyushu/J

14:20 - 14:25 *Time for room change*

**Topic** **Modelling and Numerical Methods** **Product and Process Design**

Room *Festsaal Werdenfels* *Konzertsaal Richard Strauss*

14:25 **Large-scale optimization strategies for zone configuration of simulated moving beds**  
Y. Kawajiri, L.T. Biegler, Carnegie Mellon University, Pittsburgh, PA/USA

**Success factors for CAPE in the engineering practice of a process plant contractor**  
G. Engl, A. Kröner, Linde AG, Höllriegelskreuth/D

**Operations and Control**  
*Olympiasaal*

14:25 **On the global dynamic optimization of highly nonlinear systems**  
A. Flores-Tlacuahuac, Universidad Iberoamericana, Mexico City/MEX; L.T. Biegler, Carnegie Mellon University, Pittsburgh, PA/USA

**Business Decision Support**  
*Zugspitze I+II*

**Novel continuous-time formulations for scheduling multi-stage multi-product batch plants with identical parallel units**  
 L. Yu, I.A. Karimi, National University of Singapore/SGP

14:50 **Modelling and simulation of MSF desalination process using gPROMS and neural network based physical property correlation**  
 M.S. Tanvir, I.M. Mujtaba, University of Bradford/UK

**Conceptual steady state process design in times of value based management**  
A. Wiesel, A. Polt, BASF Aktiengesellschaft, Ludwigshafen/D

14:50 **Control of thermal runaway via optimal bifurcation tailoring aided gain-scheduling feedback**  
P. Altimari, University Federico II, Naples/I; L. Russo, University of Salerno/I; E. Mancusi, University of Sannio, Benevento/I; M. di Bernardo, S. Crescitelli, University Federico II, Naples/I

**An approximate framework for large multistage batch scheduling problems focusing on bottleneck resources**  
 P.A. Marchetti, J. Cerdá, INTEC (UNL-CONICET), Santa Fe/RA

15:15 **Predictive modeling of ionic permselectivity of porous media**  
L. Seda, J. Kosek, Institute of Chemical Technology Prague/CZ

**An engineering company's approach to filling "CAPE gaps" in process simulation**  
 A. Kröner, Linde AG, Hoellriegelskreuth/D

15:15 **Static/dynamic analysis and controllability issues in reactive distillation columns**  
T. Lopez-Arenas, Technical University of Denmark, Lyngby/DK and Universidad Autónoma Metropolitana-Iztapalapa, Mexico D.F./MEX; E.S. Perez-Cisneros, Universidad Autónoma Metropolitana-Iztapalapa, Mexico D.F./MEX; R. Gani, Technical University of Denmark, Lyngby/DK

**Rigorous scheduling resolution of complex multipurpose batch plants: S-graph vs. MILP**  
S. Ferrer Nadal, Universitat Politècnica de Catalunya, Barcelona/E; T. Holczinger, University of Veszprém/H; C.A. Méndez, Universitat Politècnica de Catalunya, Barcelona/E; F. Friedler, University of Veszprém/H; L. Puigjaner, Universitat Politècnica de Catalunya, Barcelona/E

15:40 - **Coffee Break & Poster Session 2 - Topics „Operations and Control“ and „Infrastructure Systems“**

17:20

**Topic**

**Modelling and Numerical Methods**

**Product and Process Design**

**Operations and Control**

**Business Decision Support**

17:25

**A new operation mode for reactive batch distillation in middle vessel columns: start-up and operation**

I. Carmona, H. Arellano-Garcia, G. Wozny, Berlin University of Technology/D

**LCA of a spent lube oil re-refining process**

T.N. Kalnes, UOP LLC, DesPlaines, IL/USA; D.R. Shonnard, Michigan Technological University, Houghton, MI/USA; A. Schuppel, Puralube GmbH, Troglitz/D

17:25

**An optimization framework to computer-aided design of reliable measurement systems**

R. Angelini, C.A. Mendez, E. Musulin, L. Puigjaner, Universidad Politecnica de Catalunya, Barcelona/E

**Simulation based optimization for risk management in multi-stage capacity expansion**

X. Wan, GE (China) R&D Center Co., Ltd., Shanghai/PRC; J.F. Pekny, G.V. Reklaitis, Purdue University, West Lafayette, IN/USA

17:50

**Simulation of mass transfer in reactive absorption**

N. Asprion, BASF Aktiengesellschaft, Ludwigshafen/D

**Integration along the lifecycle of calcium fluoride in the fluorine industry**

A. Garea, R. Aldaco, I. Fernandez, A. Irabien, University of Cantabria, Santander/E

17:50

**Multivariate statistical batch process monitoring using dynamic independent component analysis**

H. Albazzaz, X.Z. Wang, The University of Leeds/UK

**An attainable region approach for effective production planning**

C. Sung, C.T. Maravelias, University of Wisconsin, Madison, WI/USA

18:15 -  
18:40

**Comparison of the startup of reactive distillation in packed and tray towers**

F. Forner, Technische Universität Berlin/D; M. Meyer, ENSIACET, Toulouse/F; M. Döker, Carl-von-Ossietzky-Universität, Oldenburg/D; J.-U. Repke, Technische Universität Berlin/D; J. Gmehling, Carl-von-Ossietzky-Universität, Oldenburg/D; G. Wozny, Technische Universität Berlin/D

**Design of sustainable processes: systematic generation & evaluation of alternatives**

A. Carvalho, Technical University of Denmark, Lyngby/DK and Instituto Superior Técnico, Lisboa/P; R. Gani, Technical University of Denmark, Lyngby/DK; H. Matos, Instituto Superior Técnico, Lisboa/P

18:15 -  
18:40

**Online prediction of end-of-batch product quality using phase-specific PLS models**

X.T. Doan, Institute of Chemical and Engineering Sciences, Singapore/SGP; R. Srinivasan, Institute of Chemical and Engineering Sciences and National University of Singapore/SGP

**A multistage stochastic programming approach with strategies for uncertainty reduction in the synthesis of process networks with uncertain yields**

B. Tarhan, I.E. Grossmann, Carnegie Mellon University, Pittsburgh, PA/USA

19:30

*GVC/DECHEMA PAT-Sitzung*

Wednesday, July 12, 2006

Program PSE/ESCAPE 2006

Room Festsaal Werdenfels

8:30 –  
9:20

**Keynote Lecture**

**Business decision making in the chemical industry: PSE opportunities**

R. Srinivasan, National University of Singapore and Institute of Chemical and Engineering Sciences, Singapore/SGP; I.A. Karimi, National University of Singapore/SGP; A.G. Vania, Singapore Refining Corporation, Jurong/SGP

09:20 –  
09:25

*Time for room change*

**Topic Modelling and Numerical Methods**

Room Festsaal Werdenfels

09:25

**Integration of generalized disjunctive programming with modular process simulators**

J.A. Caballero, A.O. Odjo, University of Alicante/E; I.E. Grossmann, Carnegie Mellon University, Pittsburgh, PA/USA

09:50

**Implementation of efficient logic-based techniques in the MINLP process synthesizer MIPSYN**

M. Ropotar, Z. Kravanja, University of Maribor/SLO

10:15

*Coffee Break*

**Topic Modelling and Numerical Methods**

10:45

**A global parametric programming optimisation strategy for multilevel problems**

N.P. Faisca, Imperial College London/UK; V. Dua, University College London/UK; P.M. Saraiva, University of Coimbra/P; B. Rustem, E.N. Pistikopoulos, Imperial College London/UK

**Product and Process Design**

Konzertsaal Richard Strauss

**Effective process design instruction: from simulation to plant design**

D.R. Lewin, E. Dassau, Technion, Haifa/IL; A. Goldis, Nilit, Migdal HaEmek/IL

**Optimization studies in sulfuric acid production**

A.A. Kiss, University of Amsterdam/NL; C.S. Bildea, P.J.T. Verheijen, Delft University of Technology/NL

**Product and Process Design**

**Developments in the sequential framework for Heat Exchanger Network Synthesis of industrial size problems**

R. Anantharaman, T. Gundersen, Norwegian University of Science and Technology, Trondheim/N

Konzertsaal Richard Strauss

8:30 –  
9:20

**Keynote Lecture**

**Hierarchical multiscale model-based design of experiments, catalysts, and reactors for fuel processing**

D.G. Vlachos, A.B. Mhadeshwar, N.S. Kaisare, University of Delaware, Newark, DE/USA

**Operations and Control**

Olympiasaal

09:25

**State estimation of a molten carbonate fuel cell by an extended Kalman filter**

M. Grötsch, M. Mangold, M. Sheng, MPI für Dynamik komplexer technischer Systeme, Magdeburg/D; A. Kienle, MPI für Dynamik komplexer technischer Systeme und Otto-von-Guericke-Universität Magdeburg/D

09:50

**Methods of state estimation for particulate processes**

M. Mangold, MPI für Dynamik komplexer technischer Systeme, Magdeburg/D; C. Steyer, Otto-von-Guericke-Universität, Magdeburg/D; B. Niemann, A. Voigt, MPI für Dynamik komplexer technischer Systeme, Magdeburg/D; K. Sundmacher, MPI für Dynamik komplexer technischer Systeme und Otto-von-Guericke-Universität, Magdeburg/D

**Biological Systems**

Zugspitze I+II

**Optimal delivery of chemotherapeutic agents in cancer**

P. Dua, Imperial College London/UK; V. Dua, University College London/UK; E.N. Pistikopoulos, Imperial College London/UK

**Systematic design of drug delivery therapies**

M. Xenos, L. Zhang, R.M.B. Somayaji, S. Kondapalli, A.A. Linninger, University of Illinois at Chicago, IL/USA

**Biological Systems**

10:45

**A Lab-on-a-chip simulation framework**

A.J. Pfeiffer, X. He, T. Mukherjee, S. Hauan, Carnegie Mellon University, Pittsburgh, PA/USA

**Business Decision Support**

**Application of multi-stage scheduling**

P. Bongers, B. Bakker, Unilever Food and Health Research Institute, Vlaardingen/NL



11:10	<p><b>Global bounds on optimal solutions in chemical process design</b> U.-U. Haus, Otto-von-Guericke-Universität, Magdeburg/D; J.P. Gangadwala, MPI für Dynamik Komplexer Technischer Systeme, Magdeburg/D; <u>A. Kienle</u>, MPI für Dynamik Komplexer Technischer Systeme und Otto-von-Guericke-Universität, Magdeburg/D; D. Michaels, Otto-von-Guericke-Universität, Magdeburg/D; A. Seidel-Morgenstern, MPI für Dynamik Komplexer Technischer Systeme und Otto-von-Guericke-Universität, Magdeburg/D; R. Weismantel, Otto-von-Guericke-Universität, Magdeburg/D</p>	<p><b>Structural design of polymers for membrane based separation processes using reverse simulation approach</b> <u>V. Soni</u>, J. Abildskov, G. Jonsson, R. Gani, Technical University Denmark, Lyngby/DK; N. Karayiannis, V. Mavrantzas, University of Patras/GR</p>	<p>11:10 <b>Two level control of the sequence fed batch – continuous hybridoma bioreactor</b> <u>I.D. Ofiteru</u>, A. Woinaroschy, V. Lavric, University Politehnica of Bucharest/RO</p>	<p><b>A CP method for the scheduling of multiproduct continuous plants with resource constraints</b> L.J. Zeballos, <u>G.P. Henning</u>, Universidad Nacional del Litoral, Santa Fe/RA</p>
11:35	<p><b>Towards a novel optimisation algorithm with simultaneous knowledge acquisition for distributed computing environments</b> S. Yang, A.C. Kokossis, <u>P. Linke</u>, University of Surrey, Guildford/UK</p>	<p><b>Polyurethane design using stochastic optimization</b> J.C. Eslick, <u>K.V. Camarda</u>, University of Kansas, Lawrence, KS/USA</p>	<p>11:35 <b>Solid fuel decomposition modelling for the design of biomass gasification systems</b> <u>D. Brown</u>, T. Fuchino, Tokyo Institute of Technology/J; F. Maréchal, Swiss Federal Institute of Technology, Lausanne/CH</p>	<p><b>Scheduling and planning with timed automata</b> <u>S. Panek</u>, S. Engell, O. Stursberg, University of Dortmund/D</p>
12:00 – 13:30	<i>Lunch Break</i>			
Room	<b>Festsaal Werdenfels</b>		<b>Konzertsaal Richard Strauss</b>	
13:30	<p><b>Keynote Lecture</b> <b>Process intensification and process system engineering: a friendly symbiosis</b> <u>J.A. Moulijn</u>, A. Stankiewicz, J. Grievink, Delft University of Technology/NL; <u>A. Górak</u>, University Dortmund/D</p>		<p>13:30 <b>Keynote Lecture</b> <b>The systems engineering of cellular processes</b> <u>V. Hatzimanikatis</u>, L. Wang, Northwestern University, Evanston, IL/USA</p>	
14:20 – 14:25	<i>Time for room change</i>			
Topic	<b>Modelling and Numerical Methods</b>	<b>Product and Process Design</b>	<b>Operations and Control</b>	<b>Business Decision Support</b>
Room	<i>Festsaal Werdenfels</i>		<i>Konzertsaal Richard Strauss</i>	
14:25	<p><b>Network of three catalytic reactors with periodical feed switching for methanol synthesis: bifurcation analysis</b> M. Pota, University Federico II, Napoli/I; <u>L. Russo</u>, University of Salerno, Fisciano/I; E. Mancusi, University of Sannio, Benevento/I; S. Crescitelli, University Federico II, Napoli/I;</p>	<p><b>Improved solutions for zebra mussel (Dreissena polymorpha) control – a chemical product engineering approach</b> <u>R. Costa</u>, University of Cambridge/UK; P.M. Saraiva, University of Coimbra/P; P. Elliott, D.C. Aldridge, G.D. Moggridge, University of Cambridge/UK</p>	<p>14:25 <b>A real time adaptive dynamic programming approach for planning and scheduling</b> N.E. Pratikakis, <u>J.H. Lee</u>, M.J. Realf, Georgia Institute of Technology, Atlanta, GA/USA</p>	<p><b>Workflow support for inter-organizational design processes</b> <u>R. Hai</u>, M. Heller, W. Marquardt, M. Nagl, R. Wörzberger, RWTH Aachen University/D</p>

14:50	<b>Dynamical and stationary analysis of an electrolyte diode and comparison with experiments</b> <u>Z. Slouka</u> , M. Pribyl, J. Lindner, D. Snita, M. Marek, Institute of Chemical Technology, Prague/CZ	<b>On the rapid development of new products through empirical modeling with diverse data-bases</b> <u>J.F. MacGregor</u> , K. Muteki, McMaster University, Hamilton, ONT/CDN; T. Ueda, Mitsubishi Chemical Corporation, Yokkaichi/J	14:50 <b>Simultaneous scheduling and optimization of a copper plant</b> <u>I. Harjunkoski</u> , H.W. Borchers, M. Fahl, ABB Corporate Research, Ladenburg/D	<b>A planning support system for biomass-based power generation</b> <u>N. Ayoub</u> , K.F. Wang, T. Kagiyama, H. Seki, Y. Naka, Tokyo Institute of Technology, Yokohama/J
15:15	<b>Calculation of three-phase bubble columns</b> <u>D. Wiemann</u> , Bayer Technology Services GmbH, Uerdingen/D; D. Mewes, University of Hannover/D	<b>Computer aided methodology for simultaneous synthesis, design &amp; analysis of chemical products-processes</b> <u>L. d'Anterrosches</u> , R. Gani, Technical University of Denmark, Lyngby/DK	15:15 <b>An effective MIDO approach for the simultaneous cyclic scheduling and control of polymer grade transition operations</b> <u>A. Flores-Tlacuahuac</u> , Universidad Iberoamericana, Mexico City/MEX; I.E. Grossmann, Carnegie Mellon University, Pittsburgh, PA/USA	<b>Restructuring methodology in process engineering for sustainable development</b> <u>I. Koshijima</u> , A. Shindo, Chiba Institute of Technology, Narashino/J; Y. Hashimoto, Nagoya Institute of Technology/J; T. Umeda, Aoyama Gakuin University Research Institute, Tokyo/J
15:40 – 17:20	<b>Coffee Break &amp; Poster Session 3 - Topics „Modelling and Numerical Methods“ and „Biological Systems“</b>			
<b>Topic</b>	<b>Modelling and Numerical Methods</b>	<b>Product and Process Design</b>	<b>Operations and Control</b>	<b>Business Decision Support</b>
17:25	<b>Development of a multi-compartment dynamic model for the prediction of particle size distribution and particle segregation in a catalytic olefin polymerization FBR</b> G. Dompazis, V. Kanellopoulos, <u>C. Kiparissides</u> , Aristotle University of Thessaloniki/GR	<b>Model-based optimal design of pharmaceutical formulations</b> <u>F.P. Bernardo</u> , P.M. Saraiva, S. Simões, University of Coimbra/P	17:25 <b>Multiscale analysis and monitoring of paper surface</b> <u>M.S. Reis</u> , P.M. Saraiva, University of Coimbra/P	<b>Close loop supply chains: managing product recovery portfolio</b> <u>A.C.S. Amaro</u> , Inst. Sup. Cont. Adm. – ISCAC, Coimbra/P; A.P.F.D. Barbosa-Póvoa, Instituto Superior Técnico – DEG, Lisboa/P
17:50	<b>Mixing in a T-shaped microreactor: scales and quality of mixing</b> <u>D. Bothe</u> , RWTH Aachen/D; C. Stemich, H.-J. Warnecke, University of Paderborn/D	<b>Correlation and prediction of drug molecule solubility with the NRTL-SAC model</b> <u>C.-C. Chen</u> , Aspen Technology, Inc., Cambridge, MA/USA; P.A. Crafts, AstraZeneca Pharmaceuticals Ltd., Macclesfield/UK	17:50 <b>Theoretical analysis and experimental studies of mixed product run-to-run control</b> M.-F. Wu, <u>S.-S. Jang</u> , D.S.-H. Wang, National Tsing-Hua University, Hsin-Chu/RC; Y. Zheng, Huazhong University of Science and Technology, Wuhan/PRC	<b>Lagrangian-based techniques for the supply chain management of flexible process networks</b> P. Chen, <u>J.M. Pinto</u> , Polytechnic University, Brooklyn, NY/USA
18:15 – 18:40	<b>CFD model of a semi-batch reactor for the precipitation of nanoparticles in the droplets of a microemulsion</b> A.A. Öncül, Otto-von-Guericke-University, Magdeburg/D; <u>B. Niemann</u> , MPI for Dynamics of Complex Technical Systems, Magdeburg/D; K. Sundmacher, MPI for Dynamics of Complex Technical Systems and Otto-von-Guericke-University, Magdeburg/D; D. Thévenin, Otto-von-Guericke-University, Magdeburg/D	<b>Integrating advanced thermodynamics and process and solvent design for gas separation</b> <u>E. Keskes</u> , C.S. Adjiman, A. Galindo, G. Jackson, Imperial College London/UK	18:15 – 18:40 <b>Integrating stiction diagnosis and stiction compensation in process control valves</b> R. Srinivasan, Honeywell Inc, Phoenix, AZ/USA; <u>R. Rengaswamy</u> , Clarkson University, Potsdam, NY/USA	<b>Integration of discrete-event simulation and optimization for the design of value networks</b> <u>M. Schlegel</u> , G. Brosig, A. Eckert, K. Engelke, M. Jung, A. Polt, M. Sonnenschein, C. Vogt, BASF Aktiengesellschaft, Ludwigshafen/D
19:30	<i>Conference Dinner at the Bayernhalle – sponsored by BASF Aktiengesellschaft</i>			



The Chemical Company

Thursday, July 13, 2006

Program PSE/ESCAPE 2006

Room *Festsaal Werdenfels*  
8:30 - 9:20 **Keynote Lecture**  
**Model-centric technologies for support of manufacturing operations**  
J.A. Romagnoli, Louisiana State University, Baton Rouge, LA/USA;  
P.A. Rolandi, Process Systems Enterprise Ltd., London/UK

09:20 – 09:25 *Time for room change*

Topic	Modelling and Numerical Methods	Operations and Control
Room	<i>Festsaal Werdenfels</i>	<i>Konzertsaal Richard Strauss</i>
09:25	<b>Dynamic oil and gas production optimization via explicit reservoir simulation</b> D.I. Gerogiorgis, Imperial College London/UK; G. Bowen, Schlumberger Cambridge Research (SCR) Ltd./UK; M. Georgiadis, Process Systems Enterprise (PSE) Ltd., London/UK; C.C. Pantelides, Imperial College London and Process Systems Enterprise (PSE) Ltd., London/UK; E.N. Pistikopoulos, Imperial College London/UK	<b>Stability analysis of nonlinear model predictive control: an optimization based approach</b> V. Dua, University College London/UK
09:50	<b>Multi-scale modelling and optimisation of hydrogen storage systems using advanced solid materials</b> E. Kikkinides, University of Western Macedonia, Kozani/GR; M.C. Georgiadis, Process Systems Enterprise Ltd., Themi-Thessaloniki/GR; M. Konstantakou, University of Western Macedonia, Kozani and National Center for Scientific Research "DEMOKRITOS", Athens/GR; A. Stubos, National Center for Scientific Research "DEMOKRITOS", Athens/GR	<b>Chance constrained programming approach to process optimization under uncertainty</b> P. Li, Technical University of Ilmenau/D; H. Arellano-Garcia, G. Wozny, Technical University of Berlin/D
10:15	<i>Coffee Break</i>	

*Konzertsaal Richard Strauss*

8:30 - 9:20 **Keynote Lecture**  
**Systems biology and the silicon cell: order out of chaos**  
H.V. Westerhoff, The University of Manchester/UK and Free University, Biocentre Amsterdam/NL

	Operations and Control	Biological Systems
	<i>Olympiasaal</i>	<i>Zugspitze I+II</i>
09:25	<b>Optimal current distribution control for parallel electrolytic baths</b> H. Kugemoto, K. Ozaki, Y. Kutsuwa, Sumitomo Chemical Co., Ltd., Niihama/J; Y. Hashimoto, Nagoya Institute of Technology/J	<b>Dissipative particle dynamics simulation of ibuprofen molecules distribution in the matrix of solid lipid microparticles (SLM)</b> C.X. Long, L.J. Zhang, Y. Qian, South China University of Technology, Guangzhou/PRC
09:50	<b>Systematic design of logic controllers for processing plants starting from informal specifications</b> S. Lohmann, O. Stursberg, S. Engell, University of Dortmund/D	<b>Prediction of secondary structures of proteins using a two-stage method</b> M. Turkay, O. Yilmaz, F. Uney, Koc University, Istanbul/TR

Topic	Modelling and Numerical Methods	Modelling and Numerical Methods	Operations and Control	Biological Systems
10:45	<b>A "targeted" QSPR for prediction of properties</b> N. Brauner, Tel-Aviv University/IL; R.P. Stateva, Bulgarian Academy of Sciences, Sofia/BG; G.S. Cholakov, University of Chemical Technology and Metallurgy, Sofia/BG; <u>M. Shacham</u> , Ben-Gurion University, Beer-Sheva/IL	<b>Application of particulate models for industrial processes</b> <u>G. Skillas</u> , C. Becker, M. Verduyn, J. Vorholz, Degussa AG, Hanau/D	10:45 <b>Real-time failure prediction for chemical processes: plantwide framework</b> A. Meel, <u>W.D. Seider</u> , University of Pennsylvania, Philadelphia, PA/USA	<b>An integrative systems biology approach for analyzing liver hypermetabolism</b> E. Yang, Rutgers University, Piscataway, NJ/USA; F. Berthiaume, Harvard Medical School, Boston, MA/USA; M.L. Yarmush, Rutgers University, Piscataway, NJ/USA and Harvard Medical School, Boston, MA/USA; <u>I.P. Androulakis</u> , Rutgers University, Piscataway, NJ/USA
11:10	<b>Optimization of operating conditions for ferrichrome production in a membrane bioreactor using Ustilago maydis</b> <u>A. Drews</u> , H. Arellano-Garcia, M. Wendt, M. Kraume, G. Wozny, Technische Universität Berlin/D	<b>Solution of the population balance equation using the sectional quadrature method of moments (SQMOM)</b> <u>M. Attarakih</u> , Al-Balqa Applied University, Amman/JOR; H.-J. Bart, University of Kaiserslautern/D; N.M. Faqir, University of Jordan, Amman/JOR	11:10 <b>Fault diagnosis based on support vector machines and systematic comparison to existing approaches</b> <u>I. Yélamos</u> , G. Escudero, M. Graells, L. Puigjaner, Universitat Politècnica de Catalunya, Barcelona/E	<b>Hybrid metabolic flux analysis/data-driven modelling of bioprocesses</b> <u>A. Teixeira</u> , C. Alves, Universidade Nova de Lisboa, Caparica/P; P.M. Alves, M.J.T. Carrondo, IBET/ITQB, Oeiras/P; R. Oliveira, Universidade Nova de Lisboa, Caparica/P
11:35	<b>Modelling and simulation of Fe<sub>2</sub>O<sub>3</sub>/aluminum thermite combustion: experimental validation</b> L. Duraes, University of Coimbra/P; <u>P. Brito</u> , University of Coimbra and Bragança Polytechnic Institute/P; J. Campos, A. Portugal, University of Coimbra/P	<b>Simulation of the population balance for droplet breakage in a liquid-liquid stirred tank reactor using H-matrix methods</b> <u>J. Koch</u> , MPI for Dynamics of Complex Technical Systems, Magdeburg/D; W. Hackbusch, MPI of Mathematics in the Sciences, Leipzig/D; K. Sundmacher, MPI for Dynamics of Complex Technical Systems and Otto-von-Guericke-University, Magdeburg/D	11:35 <b>Discriminant analysis and control chart for the fault detection and identification</b> <u>X. Pei</u> , Y. Yamashita, M. Yoshida, S. Matsumoto, Tohoku University, Sendai/J	<b>Rotavirus-like particle production: simulation of protein production and particle assembly</b> <u>A. Roldão</u> , H.L.A. Vieira, M.J.T. Carrondo, P.M. Alves, IBET/ITQB, Oeiras/P; R. Oliveira, FCT/UNL, Caparica/P
12:00 - 12:25	<b>Direct modelling of unit operations on molecular level</b> <u>D. Babic</u> , A. Pfennig, RWTH Aachen/D	<b>The Combined-Continuum-and-Discrete-Model (CCDM) for simulation of liquid-particle flows</b> <u>K.F. Malone</u> , B.H. Xu, M. Fairweather, University of Leeds/UK	12:00 - 12:25 <b>Support for design of user interfaces in plant operations</b> <u>X. Liu</u> , H. Kosaka, M. Noda, H. Nishitani, Nara Institute of Science and Technology, Ikoma/J	<b>Reconstruction of transcriptional regulatory networks via integer linear programming</b> J.M.S. Natali, <u>J.M. Pinto</u> , Polytechnic University, Brooklyn, NY/USA
12:25 – 13:00	<b>Closing Session</b> <b>Best Paper and Best Poster Award</b>			

**Friday, July 14, 2006      Post Conference Program PSE/ESCAPE 2006**

- 08:30 – **Workshop II**  
17:30 Modeling and Design of Crystallization Processes
- 09:00 – **Workshop I**  
17:30 Chemical Reaction Analysis: From Mechanism Discovery to Reactor Optimization
- 09:00 – **Post-Conference Tour**  
18:30 Guided Tour to Castle Neuschwanstein
- 09:30 – **Workshop III**  
17:00 What's new in gPROMS 3.0?

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