Poster Program PSE/ESCAPE 2006
Session 1, Monday, July 10, 15:40 – 17:20
„Product and Process Design" and „Business decision support"

Heat exchanger networks

1.01 **Genetic algorithms approach for retrofitting heat exchanger network with standard heat exchangers**
R. Bochenek, J.M. Jezowski, Rzeszow University of Technology/PL

1.02 **A discrete interactive graphical method for heat exchanger network synthesis**
E.S. Fraga, University College London/UK; G.W.A. Rowe, University of Dundee/UK

1.03 **An automated method for synthesizing a multi-stream heat exchanger network based on stream pseudo-temperature**
D.W. Yuan, Y. Wang, W. Xiao, P.J. Yao, Dalian University of Technology/PRC; X. Luo, W. Roetzel, University of the Federal Armed Forces Hamburg/D

1.04 **Flexible heat exchanger network design for chemical processes with operation mode changes**
M. Noda, H. Nishitani, Nara Institute of Science and Technology, Ikoma/J

1.05 **A hybrid methodology for detailed heat exchanger design in the optimal synthesis of heat exchanger networks**
J.M. García, J.M. Ponce, M. Serna, Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Michoacán/MEX

1.06 **Optimal design of shell-and-tube heat exchangers using genetic algorithms**
J.M. Ponce, M. Serna, Universidad Michoacana de San Nicolás de Hidalgo, Morelia, Michoacán/MEX; V. Rico, A. Jiménez, Instituto Tecnológico de Celaya, Guanajuato/MEX

Product design

1.07 **Optimization of nanosized silver particles synthesis via sequential pseudo-uniform design method**
J.S. Chang, Y.P. Lee, Tatung University, Taipei/RC

1.08 **Multiclass molecular knowledge framework for product and process design**
M. Korichi, Laboratoire de Génie Chimique, Toulouse/F and Université de Ouargla/DZ; V. Gerbaud, P. Floquet, Laboratoire de Génie Chimique, Toulouse/F; A.H. Meniai, Université de Constantine/DZ; S. Nacef, Université de Sétif/DZ; X. Joulia, Laboratoire de Génie Chimique, Toulouse/F

1.09 **Quantitative structure - odour relationship: using of multidimensional data analysis and neural network approaches**
M. Korichi, Laboratoire de Génie Chimique, Toulouse/F and Université de Ouargla/DZ; V. Gerbaud, P. Floquet, Laboratoire de Génie Chimique, Toulouse/F; A.-H. Meniai, Université de Constantine/DZ; S. Nacef, Université de Sétif/DZ; X. Joulia, Laboratoire de Génie Chimique, Toulouse/F

1.10 **Property clustering and group contribution for process and molecular design**
F.T. Eljack, M.R. Eden, Auburn University, AL/USA; V. Kazantzi, M.M. El-Halwagi, Texas A&M University, College Station, TX/USA

1.11 **Molecular design based on enhanced topological descriptors**
A.A. Kiss, University of Amsterdam/NL; M.V. Diudea, "Babes-Bolyai" University, Cluj-Napoca/RO

1.12 **Cooling crystallization: a process-product perspective**
C.B.B. Costa, R. Maciel Filho, State University of Campinas/BR

1.13 **Development of a mixture design methodology for problems with incomplete information. Application to PVC heat stabilisers design**
U.G. da Cruz, G.A. Carrillo Le Roux, Universidade de São Paulo/BR

1.14 **Principles for chemical products design**
L.A. Cisternas, Universidad de Antofagasta/RCH; E.D. Galvez, Northern Catholic University, Antofagasta/RCH

1.15 **Morphogenesis of polyolefin particles in polymerization reactors**
B. Horackova, J. Kosek, Institute of Chemical Technology Prague/CZ

1.16 **Optimal scheduling of tests for new product development**
H.-R. Son, S.-K. Heo, I.-B. Lee, Pohang University of Science and Technology/ROK

1.17 **Systems for decision support in industrial use**
K. Coböken, G. Mogk, T. Mrziglod, U. Telle, Bayer Technology Services GmbH, Leverkusen/D

Process design
1.18 **Simulation and optimization in 1,3-butadiene process from C$_4$-cut using genetic algorithm**
F. Jalali Farahani, R. Saffari, University of Tehran/IR

1.19 **A synthesis procedure for the design of semicontinuous reactive distillation for specialty chemicals**
T.A. Adams II, W.D. Seider, University of Pennsylvania, Philadelphia, PA/USA

1.20 **Multi-objective optimisation of batch distillation processes**
T.M. Barakat, E.S. Fraga, E. Sorensen, University College London/UK

1.21 **Sustainable production of industrial chemical products from bioresources**
J.R. Seay, Degussa Corporation, Mobile and Auburn University, AL/USA; M.R. Eden, Auburn University, AL/USA; R.N. D'Alessandro, Degussa Corporation, Mobile, AL/USA, C. Weckbecker, Degussa AG, Hanau/D

1.22 **Integration of process design and operation for chemical product development with implementation of a kilo-plant**
Y. Qian, Z.H. Wu, Y.B. Jiang, South China University of Technology, Guangzhou/PRC

1.23 **Process intensification for systematic synthesis of new distillation systems with less than N-1 columns**
B.-G. Rong, I. Turunen, Lappeenranta University of Technology/FIN

1.24 **Modeling and designing powder mixing processes utilizing compartment modeling**
P.M. Portillo, F.J. Muzzio, M.G. Ierapetritou, Rutgers University, Piscataway, NJ/USA

1.25 **Heat integration between processes: integrated structure using stage-wise model**
A. Kovac Kralj, P. Glavic, University of Maribor/SLO

1.26 **Integrative optimization of refining and petrochemical plants**
C. Li, X. He, B. Chen, Tsinghua University, Beijing/PRC; B. Chen, Z. Gong, L. Quan, PetroChina, Lanzhou/PRC

1.27 **Multi-criteria evaluation for the chemical industrial parks**
J. Xiaoping, T. Zhang, L. Shi, Tsinghua University, Beijing/PRC

Planning and scheduling
1.28 **A combinatorial formulation for optimal sizing, scheduling and shift policy in designing the milling section of a ceramic tile industrial plant**
B.P.M. Duarte, Polytechnic School of Engineering and University of Coimbra/P; L.O. Santos, University of Coimbra/P; J.S. Mariano, Polytechnic School of Engineering, Coimbra/P

1.29 **Decomposition based algorithm for the design and scheduling of multipurpose batch plants**
T. Pinto, INETI, Lisbon/P; A.P. Barbósa-Póvoa, IST, Lisbon/P; A.Q. Novais, INETI, Lisbon/P

1.30   **Scheduling of identical and parallel on/off production units under uncertainty in cost and demand prediction**
P. Pulkkinen, R. Ritala, Tampere University of Technology/FIN

1.31   **A flexible framework for optimal biorefinery product allocation**
N.E. Sammons Jr., M.R. Eden, Auburn University, AL/USA; H.T. Cullinan, Alabama Center for Paper and Bioresource Engineering, Auburn, AL/USA; L. Perine, American Forest and Paper Association/USA; E. Connor, ThermoChem Recovery International, Baltimore, MD/USA

1.32   **Medium term planning of biopharmaceutical manufacture under uncertainty**
K. Lakhdar, S.S. Farid, University College London/UK; J. Savery, BioPharm Services UK, Chesham/UK; N.J. Titchener-Hooker, L.G. Papageorgiou, University College London/UK

1.33   **A multi-criteria optimization model for planning of a supply chain network under demand uncertainty**
C.-L. Chen, T.Y. Yuan, C.-Y. Chang, W.C. Lee, Y.C. Ciou, National Taiwan University, Taipei/RC

1.34   **Strategic planning and design using MILP: an industrial application from the tissue manufacturing industry**
J. Westerlund, Åbo Akademi University, Turku/FIN; P. Castro, DMS/INETI, Lisbon/P; S. Forssell, Metsä Tissue Corporation, Mariestad/S

1.35   **Multiple time grid continuous-time formulation for the short term scheduling of multiproduct batch plants**
P. Castro, DMS/INETI, Lisbon/P; I. Grossmann, Carnegie Mellon University, Pittsburgh, PA/USA

1.36   **An inventory control scheme for simultaneous production planning and scheduling under demand uncertainty**
T. Nishi, H. Tominaga, M. Konishi, Okayama University/J

1.37   **Implementation of an integrated platform of process system operations for education and research**
X.X. Li, Y. Qian, Y.B. Jiang, South China University of Technology, Guangzhou/PRC

1.38   **Integration of multi-scale planning and scheduling problems**
H. Stefansson, Imperial College London/UK; P. Jensson, University of Iceland, Reykjavik/IS; N. Shah, Imperial College London/UK

1.39   **Plant-wide planning and marginal value analysis for a refinery complex**
W. Li, Hong Kong University of Science and Technology/PRC; X. Liang, PetroChina Company Limited, Daqing/PRC; C. Hui, Hong Kong University of Science and Technology/PRC

1.40   **Refinery planning under correlated and truncated price and demand uncertainties**
W. Li, I.A. Karimi, R. Srinivasan, National University of Singapore/SGP

1.41   **Pipeline scheduling and distribution centre management - a real-world scenario at CLC**
S. Relvas, A.P.F.D. Barbosa-Póvoa, H.A. Matos, Instituto Superior Técnico, Lisbon/P; J. Fialho, A.S. Pinheiro, Companhia Logística de Combustíveis, Aveiras de Cima/P

1.42   **Scheduling under demand uncertainty using a new multiparametric programming approach**
Z. Jia, M.G. Ierapetritou, Rutgers University, Piscataway, NJ/USA

1.43   **Planning and scheduling of multipurpose continuous plants**
C. Schwindt, S. Herrmann, Technical University of Clausthal/D; N. Trautmann, University of Bern/CH

1.44   **Priority-rule based scheduling of chemical batch processes**
N. Trautmann, University of Bern/CH; C. Schwindt, Technical University of Clausthal/D

1.45   **A rigorous approach to coordinate production and transport scheduling in a multi-site system**
C.A. Mendez, A. Bonfill, A. Espuna, L. Puigjaner, Universidad Politecnica de Catalunya, Barcelona/E

1.46   **Scheduling with high accuracy at low maintenance costs: an approach using discrete event simulation**
M. Jung, C. Vogt, BASF Aktiengesellschaft, Ludwigshafen/D

1.47   **An integrated model for planning in global chemical supply chains**
A. Sundaramoorthy, Institute of Chemical and Engineering Sciences, Singapore/SGP; S. Xianming, I.A. Karimi, National University of Singapore/SGP; R. Srinivasan, National University of Singapore and Institute of Chemical and Engineering Sciences, Singapore/SGP

1.48   **A hybrid approach using CLP and MILP applied to tank farm operation scheduling**
S.L. Stebel, F. Neves Jr., L.V.R. Arruda, Centro Federal de Educação Tecnológica do Paraná/BR

1.49   **Efficient MILP-based solution strategies for large-scale industrial batch scheduling problems**
P. Castro, INETI, Lissabon/P; C. Méndez, UPC, Barcelona/E; I. Grossmann, Carnegie Mellon University, Pittsburgh, PA/USA; I. Harjunkoski, M. Fahl, ABB Corporate Research, Ladenburg/D

Distillation columns

1.50   **Importance of the selection of feed tray location on the optimum design of a heterogeneous azeotropic distillation column with p-xylene feed impurity**
I.L. Chien, National Taiwan University of Science and Technology, Taipei/RC; H.Y. Lee, T.K. Gau, H.P. Huang, National Taiwan University, Taipei/RC

1.51   **Mixed-integer optimization of distillation column tray positions in industrial practice**
I. Thomas, A. Kröner, Linde AG, Höllriegelskreuth/D

1.52   **Synthesis of separation systems for azeotropic mixtures: preferred distillation region**
S.K. Wasylkiewicz, Aspen Technology, Inc., Calgary, ALTA/CDN

1.53   **Design and control of homogeneous and heterogeneous reactive distillation for ethyl acetate process**
H.-Y. Lee, H.-P. Huang, National Taiwan University, Taipei/RC; I.-L. Chien, National Taiwan University of Science and Technology, Taipei/RC

1.54   **Feasibility study of batch reactive distillation in hybrid columns**
C. Steger, E. Rev, Z. Fonyo, Budapest University of Technology/H; M. Meyer, ENSIACET, Toulouse/F; Z. Lelkes, Budapest University of Technology/H

1.55   **Generic model framework for the synthesis of structured reactive separation processes**
G. Sand, M. Tylko, S. Barkmann, G. Schembecker, S. Engell, Universität Dortmund/D

1.56   **Mathematical development for scaling-up of molecular distillators: strategy and test with recovering carotenoids from palm oil**
C.B. Batistella, E.B. Moraes, R. Maciel Filho, M.R. Wolf-Maciel, State University of Campinas/BR

Environment, health and safety

1.57 **Supporting waste minimization studies by integrating expert system with process simulators**
I. Halim, Institute of Chemical and Engineering Sciences, Singapore/SGP; R. Srinivasan, Institute of Chemical and Engineering Sciences and National University of Singapore/SGP

1.58 **A chemical process design framework including different stages of environmental, health and safety (EHS) assessment**
H. Sugiyama, U. Fischer, ETH Zürich/CH; M. Hirao, University of Tokyo/J; K. Hungerbühler, ETH Zürich/CH

1.59 **A knowledge-based approach for accident information retrieval**
M. Suzuki, R. Batres, Toyohashi University of Technology/J; T. Fuchino, Tokyo Institute of Technology/J; Y. Shimada, National Institute of Industrial Safety, Tokyo/J; P.W. Chung, Loughborough University/UK

1.60 **Knowledge extraction during the design of activated sludge systems**
X. Flores, M. Poch, I. Rodriguez-Roda, Universitat de Girona/E; L. Jimenez, Universitat de Barcelona/E; R. Banares-Alcantara, University of Oxford/UK

1.61 **Case study on design of regulatory policies for sustainable emission reduction**
A. Malcolm, L. Zhang, A.A. Linninger, University of Illinois at Chicago, IL/USA

1.62 **A decomposition/reconstruction algorithmic procedure for computer aided case based reasoning - implementation in biodegradation**
F.A. Batzias, University of Piraeus/GR

1.63 **Environmentally conscious design of ethanol fed fuel cell system**
L. Hernández, V. Kafarov, Industrial University of Santander, Bucaramanga/CO

1.64 **Modelling and design of a biochemical process for NOx removal**
C.S. Bildea, M.L. Oudshoorn, C. Picioreanu, Delft University of Technology/NL; A.C. Dimian, University of Amsterdam/NL

1.65 **Multicriteria design of separation sequences by including HSE criteria and uncertainty**
K. Cziner, M. Hassim, M. Hurme, Helsinki University of Technology, Espoo/FIN

Chemical reactors

1.66 **Effects of catalyst activity profiles on the scale-up of polymerization reactors**
S. Nemeth, J. Abonyi, B. Feil, P. Arva, University of Veszprem/H; J. Tolveth, A. Janecska, G. Nagy, TVK Ltd, Tiszaujvaros/H

1.67 **A systematic approach for automated reaction network generation**
S.-H. Hsu, B. Krishnamurthy, P. Rao, C. Zhao, S. Jagannathan, J. Caruthers, V. Venkatasubramanian, Purdue University, West Lafayette, IN/USA

1.68 **Multi-objective reactor network synthesis for industrial mass transfer limited processes**
F.J.M. Neves, D.C.M. Silva, N.M.C. Oliveira, University of Coimbra/P; F.P. Mendes, Quimigal, S.A., Estarreja/P

1.69 **Pharmaceutical process development applying automated laboratory reactors**
T. Chovan, University of Veszprem/H; I. Markovits, B. Farkas, K. Nagy, EGIS Pharmaceuticals Ltd., Budapest/H; L. Nagy, University of Veszprem/H; K. Nyíri, EGIS Pharmaceuticals Ltd., Budapest/H; F. Szeifert, University of Veszprem/H

Supply chain design

1.70 **Addressing the design of chemical supply chains under demand uncertainty**
G. Guillén, F.D. Mele, A. Espuña, L. Puigjaner, Universitat Politècnica de Catalunya, Barcelona/E

1.71   **A flexible design of logistic network against uncertain demands through hybrid meta-heuristic method**
Y. Shimizu, S. Matsuda, T. Wada, Toyohashi University of Technology/J

1.72   **An integrated model for the design and planning of supply chains with product return**
M.I. Salema, FCT-UNL, Caparica/P; A.P. Barbosa-Póvoa, CEG-IST, Lisboa/P; A.Q. Novais, INETI, Lisboa/P

1.73   **Decentralized supply chain dynamics and the quantity flexibility contract**
V. Subramanian, Oracle Corporation, Cambridge, MA/USA; J.F. Pekny, G.V. Reklaitis, Purdue University, West Lafayette, IN/USA

1.74   **A novel combined approach for supply chain modeling and analysis**
F.D. Mele, C.A. Mendez, A. Espuña, L. Puigjaner, Universitat Politecnica de Catalunya, Barcelona/E

1.75   **Multiobjective multiproduct batch plant design under uncertainty**
A. Dietz, CNRS, Nancy/F; A. Aguilar-Lasserre, C. Azzaro-Pantel, L. Pibouleau, S. Domenech, CNRS, Toulouse/F

Information technology
1.76   **Optimization-based root cause analysis**
E. Dassau, D.R. Lewin, Technion, Haifa/IL

1.77   **A view-based information model for enterprise integration in process industries**
P. Li, South China University of Technology, Guangzhou/PRC; M.L. Lu, Aspen Technology Inc., Cambridge, MA/USA; Y.S. Peng, B. Hua, South China University of Technology, Guangzhou/PRC

1.78   **Information modeling for pharmaceutical product development**
C. Zhao, L. Hailemariam, A. Jain, G. Joglekar, V. Venkatasubramanian, K. Morris, G. Reklaitis, Purdue University, West Lafayette, IN/USA

1.79   **Information sharing in a distributed enterprise: impact on supply chain performance and decision-making**
I.B. Owusu, S. Hauan, Carnegie Mellon University, Pittsburgh, PA/USA

1.80   **Integration of supply chain management and logistics: development of an electronic data interchange for SAP servers**
L. Jiménez-Esteller, University of Barcelona/E; R. Muñoz, Qualitas Information Systems, Barcelona/E

1.81   **PRoduct ONTOlogy. Defining product-related concepts for production planning activities**
D.M. Giménez, UNL, Santa Fe/RA; M.M. Vegetti, Universidad Tecnologica Nacional, Santa Fe/RA; G.P. Henning, UNL, Santa Fe/RA; H.P. Leone, Universidad Tecnologica Nacional, Santa Fe/RA

1.82   **Recipe informatics to shorten the lead time from product development to production in batch processes**
T. Fuchino, Tokyo Institute of Technology/J; T. Kitajima, Tokyo University of Agriculture and Technology/J; Y. Shimada, National Institute of Industrial Safety, Tokyo/J; K. Takeda, Shizuoka University, Hamamatsu/J; S. Hashizume, Nagoya University/J; T. Hamaguchi, Nagoya Institute of Technology/J; R. Batres, Toyohashi University of Technology/J; A. Yamada, Mitubishi Chemical Co. Ltd., Yokkaichi/J; K. Kawano, Mitsui Chemicals, Inc. Oomuta/J; Y. Hashimoto, Nagoya Institute of Technology/J

1.83   **Innovation and knowledge management: using the combined approach TRIZ-CBR in process system engineering**
G. Cortes Robles, S. Negny, J.M. Le Lann, ENSIACET, Toulouse/F

1.84 **Decision-making tool for scheduling of batch processes: the dynamic hybrid simulation kernel**
N. Olivier, <u>R. Thery</u>, G. Hétreux, J.M. Le Lann, Laboratoire de Génie Chimique, Toulouse/F

Poster Program PSE/ESCAPE 2006
Session 2, Tuesday, July 11, 15:40 – 17:20
„Operations and Control" and „Infrastructure Systems"

Plant wide control

2.01 **Branch and bound methods for control structure design**
<u>V. Kariwala</u>, S. Skogestad, Norwegian University of Science and Technology, Trondheim/N

2.02 **A thermodynamic based plant-wide control design procedure of the Tennessee Eastman process**
<u>L.T. Antelo</u>, I. Otero-Muras, J.R. Banga, A.A. Alonso, Instituto de Investigaciones Marinas-CSIC, Vigo/E

2.03 **Using the process schematic in plant-wide disturbance analysis**
S.Y. Yim, H.G. Ananthakumar, L. Benabbas, University College London/UK; A. Horch, R. Drath, ABB Corporate Research Centre, Ladenburg/D; <u>N.F. Thornhill</u>, University College London/UK

2.04 **Simulation based engineering - from process engineering to automation engineering**
H. Fischer, Siemens AG, Erlangen/D; <u>J.C. Toebermann</u>, Siemens AG, Aachen/D

2.05 **Degrees of freedom analysis for process control**
<u>M. Rodriguez</u>, J.A. Gayoso, Universidad Politecnica de Madrid/E

Process monitoring and supervision

2.06 **Multiscale SPC in the presence of multiresolution data**
<u>M.S. Reis</u>, P.M. Saraiva, University of Coimbra/P

2.07 **Using multi sensor data fusion for level estimation in a separator**
<u>N.-O. Skeie</u>, Telemark Technological R&D Centre, Porsgrunn/N; S. Mylvaganam, B. Lie, Telemark University College, Porsgrunn/N

2.08 **Product quality estimation using multi-rate sampled data**
<u>B. Lin</u>, Technical University of Denmark, Lyngby/DK; B. Recke, T.V. Jensen, J. Knudsen, FLSmidth Automation, Valby/DK; S.B. Jørgensen, Technical University of Denmark, Lyngby/DK

2.09 **An integrated framework based on data driven techniques for process supervision**
<u>B. Bhushan</u>, University of Sydney/AUS; J.A. Romagnoli, Louisiana State University, Baton Rouge, LA/USA

2.10 **Automatic adjustment of data compression in process information management systems**
F. Alsmeyer, AixCAPE e.V., Aachen/D

2.11 **Adaptive monitoring statistics based on state space updating using canonical variate analysis**
<u>L. Changkyu</u>, S.W. Choi, I.-B. Lee, Pohang University of Science and Technology/ROK

2.12 **Optimal configuration of artificial neural networks**
V. Dua, University College London/UK

Estimation and control

2.13 **Nonlinear model predictive control of the wastewater treatment plant**
<u>M.V. Cristea</u>, S.P. Agachi, "Babes-Bolyai" University of Cluj-Napoca/RO

2.14 **Constrained control for chemical processes using reference governor**
K. Kogiso, M. Noda, H. Nishitani, Nara Institute of Science and Technology, Ikoma/J

2.15 **Improving observability of large-scale systems by iterative weighting adjustment**
R. Faber, H. Arellano-Garcia, Technical University of Berlin/D; P. Li, Technical University of Ilmenau/D; G. Wozny, Technical University of Berlin/D

2.16 **Application of a hybrid control approach to highly nonlinear chemical processes**
Y. Sakakura, M. Noda, H. Nishitani, Nara Institute of Science and Technology, Ikoma/J; Y. Yamashita, M. Yoshida, S. Matsumoto, Tohoku University, Sendai/J

2.17 **Combined nonlinear model predictive control and moving horizon estimation for a copolymerisation process**
M. Diehl, P. Kuehl, H.G. Bock, J.P. Schloeder, University of Heidelberg/D; B. Mahn, BASF Aktiengesellschaft, Ludwigshafen/D; J. Kallrath, BASF Aktiengesellschaft, Ludwigshafen/D and University of Florida, Gainesville, FL/USA

2.18 **Thermodynamic diagram based estimation structure design for ternary distillation column**
A. Pulis, Universita di Cagliari/I; C. Fernandez, Universidad Autonoma Metropolitana-Itzapalapa, Mexico City/MEX; R. Baratti, Universita di Cagliari/I; J. Alvarez, Universidad Autonoma Metropolitana-Itzapalapa, Mexico City/MEX

2.19 **On-line data reconciliation and parameter estimation for an industrial polypropylene reactor**
D.M. Prata, J.C. Pinto, E.L. Lima, Universidade Federal do Rio de Janeiro/BR

2.20 **Optimal steady-state transitions under constrained predictive control**
D.K. Lam, C.L.E. Swartz, McMaster University, Hamilton, ONT/CDN

2.21 **Advances and future directions in morphology monitoring and control of organic crystals grown from solution**
X.Z. Wang, K.J. Roberts, J. Calderon De Anda, The University of Leeds/UK

2.22 **Molecular weight control in acrylonitrile polymerization with neural network based controllers**
I. Atasoy, M. Yuceer, R. Berber, Ankara University/TR

2.23 **A new approach to chance constrained process optimization and control under time-dependent uncertainties**
H. Arellano-Garcia, T. Barz, W. Martini, G. Wozny, Berlin University of Technology/D

Batch process control
2.24 **A mathematical programming approach including flexible recipes to batch operation rescheduling**
S. Ferrer-Nadal, C.A. Méndez, M. Graells, L. Puigjaner, Universitat Politècnica de Catalunya , Barcelona/E

2.25 **Reliable multi-objective optimal control of batch processes based on stacked neural network models**
A. Mukherjee , J. Zhang, University of Newcastle, Newcastle upon Tyne/UK

2.26 **Stochastic optimal control in batch reactive systems: developments on engineering applications of real option theory**
V. Rico-Ramirez, J.F. Cambero-Benitez, H. Cañada-Jaime, Instituto Tecnologico de Celaya/MEX; S. Hernandez-Castro, Universidad de Guanajuato/MEX

2.27 **A novel solution approach for quality-based retrimming optimization**
I. Harjunkoski, M. Fahl, ABB Corporate Research, Ladenburg/D

2.28 **A web service based online optimization and monitoring system for chemical processing systems**
X.Y. Li, X.X. Li, Y. Qian, South China University of Technology, Guangzhou/PRC

2.29 **An application of metamodels for process optimization**
M.V.C. Gomes, PETROBRAS S.A., Rio de Janeiro/BR; I.D.L. Bogle, University College London/UK; D. Odloak, Universidade de São Paulo/BR; E.C. Biscaia Jr., Universidade Federal do Rio de Janeiro/BR

2.30 **Large-scale dynamic optimization of an integrated cryogenic process**
M.A. Rodriguez, M.S. Diaz, Universidad Nacional del Sur, Bahia Blanca/RA

2.31 **Scheduling of storage and transfer tasks in oil refinaries by using fuzzy optimization**
L.C. Felizari, R. Lüders, Centro Federal de Educação Tecnológica do Paraná, Curitiba/BR

2.32 **Dynamic optimization of dead-end membrane filtration**
B. Blankert, B.H.L. Betlem, B. Roffel, University of Twente, Enschede/NL

2.33 **Virtual plant, new paradigm for future production management**
H.A. Gabbar, K. Nishiyama, I. Shingo, T. Ooto, K. Suzuki, Okayama University/J

2.34 **Scheduling of make and pack plants: a case study**
C.-U. Fündeling, University of Karlsruhe/D; N. Trautmann, University of Bern/CH

2.35 **Optimal operation of a mixed fluid cascade LNG plant**
J.B. Jensen, S. Skogestad, NTNU, Trondheim/N

2.36 **Optimal reactive scheduling of multipurpose, make-to-order industries**
M.C. Gomes, A. Barbosa-Póvoa, Instituto Superior Técnico, Lisboa/P; A.Q. Novais, INETI-DMS, Lisboa/P

Fault diagnosis and process safety
2.37 **Agent-based diagnosis for granulation processes**
R. Lakner, University of Veszprem/H; E. Nemeth, University of Veszprem and Computer and Automation Research Institute, Budapest/H; K.M. Hangos, Computer and Automation Research Institute, Budapest/H; I.T. Cameron, University of Queensland, Brisbane/AUS

2.38 **Fault detection and diagnosis of pulp mill process**
G. Lee, Chungju National University/ROK; T. Tosukhowong, J.H. Lee, Georgia Institute of Technology, Atlanta, GA/USA

2.39 **Graphical modeling for the safety verification of chemical processes**
J.K. Kim, Y. Lee, I. Moon, Yonsei University, Seoul/ROK

2.40 **Detection of abnormal alumina feed rate in aluminium electrolysis cells using state and parameter estimation**
K. Hestetun, M. Hovd, Norwegian University of Science and Technology, Trondheim/N

Process dynamics
2.41 **Controllability analysis of thermally coupled distillation sequences for five-component mixtures**
M. Carrera-Rodríguez, M. Ledezma-Martínez, J.G. Segovia-Hernández, S. Hernández, Universidad de Guanajuato/MEX

2.42 **Time scale separation and the link between open-loop and closed-loop dynamics**
A.C.B. de Araujo, Norwegian University of Science and Technology, Trondheim/N; M. Baldea, University of Minnesota, Minneapolis, MN/USA; S. Skogestad, Norwegian University of Science and Technology, Trondheim/N; P. Daoutidis, Aristotle University of Thessaloniki/GR

2.43 **Autothermal reactors for hydrogen production: dynamics and model reduction**
M. Baldea, University of Minnesota, Minneapolis, MN/USA; P. Daoutidis, University of Minnesota, Minneapolis, MN/USA and Aristotle University of Thessaloniki/GR

2.44 **Multiplicity of steady states in an UOP FCC unit with high efficiency regenerator**
J.L. Fernandes, C.I.C. Pinheiro, Instituto Superior Técnico, Lisboa/P; N. Oliveira, Universidade de Coimbra/P; F. Ramôa Ribeiro, Instituto Superior Técnico, Lisboa/P

Control performance monitoring
2.45 **Performance assessment and controller design for unknown systems based on gain and phase margins using modified relay feedback**
J.C. Jeng, H.P. Huang, National Taiwan University, Taipei/RC

2.46 **Diagnosis of oscillations in process control loops**
Y. Yamashita, Tohoku University, Sendai/J

Waste processing systems
2.47 **Modelling and simulation of a tyre gasification plant for synthesis gas production**
N.R. Mitta, S. Ferrer-Nadal, A.M. Lazovic, J.F. Perales, E. Velo, L. Puigjaner, Universitat Politècnica de Catalunya, Barcelona/E

2.48 **Case study of a regional network for the recovery of hazardous materials**
J. Duque, INETI, Lisboa/P; A.P.F.D. Barbosa-Póvoa, CEG-IST, Lisboa/P; A.Q. Novais, INETI, Lisboa/P

2.49 **Optimisation of a pertraction process for wastewater treatment and copper recovery**
A.M. Eliceche, Universidad de Cantabria, Santander/E; M.F. Orlandi, Universidad Nacional del Sur, Bahía Blanca/RA; A.M. Urtiaga, I. Ortiz, Universidad de Cantabria, Santander/E

Energy systems
2.50 **Library for modeling and simulating the thermal dynamics of buildings**
J.I. Videla, B. Lie, Telemark University College, Porsgrunn/N

2.51 **Data-centric demand forecasting for utilities**
Z. Beran, K. Marik, P. Stluka, Honeywell Inc., Prague/CZ

2.52 **Synergy analysis of collaboration with biofuel use for environmentally conscious energy systems**
M. Turkay, A. Soylu, Koc University, Istanbul/TR

2.53 **Operational optimization of the thermoelectric system of an oil refinery**
S.R. Micheletto, Petrobras-Petroleo S.A., São Paulo/BR; J.M. Pinto, Polytechnic University, Brooklyn, NY/USA

2.54 **Simulation of electricity production systems in autonomous networks in order to maximize the wind energy penetration**
J.K. Kaldellis, E. Kondili, Technological Educational Institute of Piraeus, Athens/GR

2.55 **Heat integration in micro-fluidic devices**
T. Zhelev, University of Limerick/IRL; O. Strelow, University of Giessen-Freiberg/D

2.56 **Network synthesis for a district energy system: a step towards sustainability**
C. Weber, Ecole Polytechnique Fédérale de Lausanne/CH; I. Heckl, F. Friedler, University of Veszprem/H; F. Maréchal, D. Favrat, Ecole Polytechnique Fédérale de Lausanne/CH

Water systems
2.57 **A new method for designing water network based on variable removal ratio of treatment process**
L. Song, J. Du, S.B. Cai, P.J. Yao, Dalian University of Technology/PRC

2.58   **Environmental life cycle impact and cost minimization in the steam and power generation plant**
P. Martinez, A.M. Eliceche, Universidad Nacional del Sur, Bahía Blanca/RA

2.59   **Cost versus network length criteria in water network optimal design**
P. Iancu, V. Plesu, University Politehnica of Bucharest/RO; V. Lavric, University Politehnica of Bucharest/RO and Vrije Universiteit Brussels/B

2.60   **Water reuse: a successful almost zero discharge case**
R.M.B. Alves, R. Guardani, A.E. Bresciani, University of São Paulo/BR; L. Nascimento, Polibrasil Resinas S.A./BR; C.A.O. Nascimento, University of São Paulo/BR

2.61   **Model development for the optimal water systems planning**
E. Kondili, J.K. Kaldellis, Technological Educational Institute of Piraeus, Athens/GR

Production systems
2.62   **A screening tool for exploring production chains**
L. Stougie, R.M. Stikkelman, M. Houwing, Delft University of Technology/NL

2.63   **Process optimization and scheduling of parallel furnaces shutdown in large-scale plants**
E. Schulz, A. Bandoni, M.S. Diaz, Universidad Nacional del Sur, Bahia Blanca/RA

Poster Program PSE/ESCAPE 2006
Session 3, Wednesday, July 12, 15:40 – 17:20
„Modelling and Numerical Methods" and „Biological Systems"
Modelling for safety analysis
3.01   **Modelling of self-ignition and process upsets in industrial gaseous hydrocarbon oxidation processes**
H.J. Pasman, Delft University of Technology/NL; M. Fairweather, University of Leeds/UK

3.02   **Automatic generation of reduced reaction mechanisms for hydrocarbon oxidation with application to autoignition boundary prediction for explosion hazards mitigation**
R. Porter, M. Fairweather, J.F. Griffiths, K.J. Hughes, A.S. Tomlin, University of Leeds/UK

3.03   **Combining HAZOP with dynamic process model development for safety analysis**
S. Eizenberg, M. Shacham, Ben-Gurion University, Beer-Sheva/IL; N. Brauner, Tel-Aviv University/IL

Optimization methods
3.04   **A simplex search method for experimental optimization with multiple objectives**
E.C. Martinez, Universidad Tecnológica Nacional, Santa Fe/RA

3.05   **A hybrid global optimization scheme for process design and dynamic optimization**
C.-T. Chen, S.-T. Peng, Feng Chia University, Taichung/RC; Y.-J. Ciou, C.-L. Chen, National Taiwan University, Taipei/RC

3.06   **Methodology for decision support among conflicting objectives using process simulators**
N. Ramzan, W. Witt, BTU-Cottbus/D

3.07   **Monitoring and improving LP optimization with uncertain parameters**
D. Zyngier, T. Marlin, McMaster University, Hamilton, ONT/CDN

3.08   **An integrated stochastic method for global optimization of continuous functions**
M. Srinivas, G.P. Rangaiah, National University of Singapore/SGP

3.09 **Strategy and framework for solving signal-based MIDO problems**
R.H. Nyström, I. Harjunkoski, ABB Corporate Research, Ladenburg/D; R. Franke, ABB AG, Mannheim/D

3.10 **Utility systems operational planning optimization based on pipeline network simulation**
X.L. Luo, B. Hua, B.J. Zhang , South China University of Technology, Guangzhou/PRC; M.L. Lu, Aspen Technology Inc., Cambridge, MA/USA

3.11 **Particle swarm for the dynamic optimization of biochemical processes**
J. Zhang, L. Xie, S. Wang, Zhejiang University, Hangzhou/PRC

3.12 **A-priori identification of critical points for the design and synthesis of flexible process schemes**
Z. Novak Pintaric, Z. Kravanja, University of Maribor/SLO

3.13 **Using water cascade analysis to synthesize water use network in batch process**
S.G. Wang, S.Q. Zheng, X. Yang, Y.G. Li, Qingdao University of Science and Technology/PRC

3.14 **Pricing utilities for large-scale chemical production site**
K. Hirata, P. Chan, H. Sakamoto, Mitsubishi Chemical Corporation, Yokkaichi/J; D.C.W. Hui, Hong Kong University of Science and Technology/PRC

3.15 **The complex distillation column network systematic optimization by mathematical programming**
S. Choi, H. Kim, C. Han, E. Yoon, Seoul National University/ROK

3.16 **Solving MINLP containing noisy variables and black-box functions using branch-and-bound**
E. Davis, M. Ierapetritou, Rutgers University, Piscataway, NJ/USA

3.17 **An approach to implicit modelling for complex process optimization**
X.G. Yuan, W.Z. An, Y.L. Liu, Y.Q. Luo, C.J. Liu, Tianjin University/PRC

Heat transfer modelling
3.18 **A heat transfer model of a scraped surface heat exchanger for ice cream**
P. Bongers, Unilever Food and Health Research Institute, Vlaardingen/NL

3.19 **Modeling of heat transfer processes in particulate systems**
Z. Süle, C. Mihálykó, B.G. Lakatos, University of Veszprém/H

3.20 **Modelling and dynamic simulation of thermal stresses in brazed plate-fin heat exchanger**
F. Picard, INP-ENSIACET, Toulouse/F and Nordon Cryogenie S.A., Golbey/F; D. Averous, Nordon Cryogenie S.A., Golbey/F; X. Joulia, D. Barreteau, INP-ENSIACET, Toulouse/F

3.21 **Numerical simulation of micro roughness effects on convective heat transfer**
S. Scholl, W. Augustin, Technical University of Braunschweig/D

Model identification
3.22 **Parameter identifiability analysis and model fitting of a biological wastewater model**
Q. Chai, Telemark University College, Porsgrunn/N; S.H. Amrani, BioTek AS, Porsgrunn/N; B. Lie, Telemark University College, Porsgrunn/N

3.23 **Grey-box stochastic modelling of industrial fed-batch cultivation**
J.K. Rasmussen, H. Madsen, S.B. Jørgensen, Technical University of Denmark, Lyngby/DK

3.24 **Optimal experimental design for the precision of a subset of model parameters in process development**
A. Yang, E.B. Martin, G. Montague, A.J. Morris, University of Newcastle/UK

3.25   **Identification of parametric and structural models based on RTD theory via GAMS package**
S. Hocine, L. Pibouleau, C. Azzaro-Pantel, S. Domenech, Laboratoire de Génie Chimique, Toulouse/F

3.26   **Model discrimination and parameter estimation through sensitivity analysis**
M. Sales-Cruz, R. Gani, Technical University of Denmark, Lyngby/DK

Modelling for design
3.27   **Assessing the performance of batch reactive distillations through conceptual models**
J. Espinosa, CONICET, Santa Fe/RA

3.28   **Process design using ionic liquids: physical property modeling**
A.E. Ayala, L.D. Simoni, Y. Lin, J.F. Brennecke, M.A. Stadtherr, University of Notre Dame, IN/USA

3.29   **Integrated design of energy-saving chemical process systems: strategy, methods and implementation**
G.M. Ostrovsky, Y.M. Volin, Karpov Institute of Physical Chemistry, Moscow/RUS;
D.S. Dvoretsky, S.I. Dvoretsky, Tambov State Technical University/RUS

3.30   **Generic hybrid models of solvent-based reactive systems combined with membrane separation system**
P.T. Mitkowski, G. Jonsson, R. Gani, Technical University of Denmark, Lyngby/DK

3.31   **Hybrid modeling for continuous production of bioethanol**
E. Ccopa Rivera, I. Mantovaneli, A.C. da Costa, R. Maciel Filho, University of Campinas/BR

3.32   **Energy saving in distillation columns: the Linde column revisited**
G. Soave, S. Donato Milanese/I; L. Pellegrini, D. Barbatti, N. Susani, S. Bonomi, Politecnico di Milano/I

Modelling methodologies and tools
3.33   **The ProMoT/Diana simulation environment**
M. Krasnyk, K. Bondareva, O. Milokhov, MPI Dynamics of Complex Technical Systems, Magdeburg/D; K. Teplinsky, National Technical University of Donetsk/UA; M. Ginkel, A. Kienle, MPI Dynamics of Complex Technical Systems and Otto-von-Guericke-University, Magdeburg/D

3.34   **"Smart models" - a framework for adaptive multi-scale modelling**
E. Fraga, University College London/UK; G. Wills, Southampton University/UK; M. Fairweather, University of Leeds/UK; T. Perris, Consultant, Woking/UK

3.35   **An agent-oriented architecture for modeling and optimization of naphtha pyrolysis process**
X. Gao, B. Chen, X. He, Tsinghua University, Beijing/PRC

3.36   **On model portability**
H.A. Preisig, T. Haug-Warberg, B.T. Loevfal, Norwegian University of Science and Technology, Trondheim/N

3.37   **Multiobjective optimization of multipurpose batch plants using superequipment class concept**
A. Mosat, L. Cavin, U. Fischer, K. Hungerbühler, ETH Zürich/CH

Reactor modelling
3.38   **Computer aided forecast of catalytic activity in an hydrotreating industrial process using artificial neural network, fuzzy logic and statistics tools**
F.Y. Jiménez, V. Kafarov, Industrial University of Santander, Bucaramanga/CO; M.L. Nuñez, Colombian Institute of Petroleum, Piedecuesta/CO

3.39   **A framework for modeling particle size effects in emulsion polymerization systems using computational fluid dynamics linked to a detailed population balance model**
R.C. Elgebrandt, D.F. Fletcher, V.G. Gomes, University of Sydney/AUS; J.A. Romagnoli, University of Sydney/AUS and Louisiana State University, Baton Rouge, LA/USA

3.40   **Modelling and simulation of coal and petcoke gasification in a co-current flow reactor**
E.M. Lopez, V.J. Garza, J. Acevedo, ITESM, Monterrey/MEX

3.41   **A comprehensive investigation on high-pressure LDPE manufacturing: dynamic modelling of compressor, reactor and separation units**
A. Baltsas, P. Pladis, Chemical Process Engineering Research Institute, Thessaloniki/GR; C.A. Kiparissides, Aristotle University of Thessaloniki/GR

3.42   **Modelling and simulation of high pressure industrial autoclave polyethylene reactor**
E. Caliani, State University of Campinas/BR; M. Cavalcanti, Politeno Industria e Comercio, Camacari/BR; F.A.N. Fernandes, Universidade Federal do Ceara, Fortaleza/BR; L.M.F. Lona, State University of Campinas/BR

3.43   **Computer aided modeling for hydrodesulfurization, hydrodenitrogenation and hydrodearomatization simultaneous reactions in a hydrotreating industrial process**
F. Jiménez, V. Kafarov, Industrial University of Santander, Bucaramanga/CO; M. Nuñez, Colombian Petroleum Institute, Piedecuesta/CO

Solids process modelling
3.44   **On the numerical calibration of discrete element models for the simulation of bulk solids**
T. Groeger, Itasca Consultants GmbH, Gelsenkirchen/D; A. Katterfeld, Universität Magdeburg/D

3.45   **Sensitivity analysis in the simulation of complex solids processes**
D. Schwier, A. Püttmann, E.-U. Hartge, G. Gruhn, J. Werther, Technical University Hamburg-Harburg/D

Separations modelling
3.46   **Validation of a digital packing algorithm for the packing and subsequent fluid flow through packed columns**
R. Caulkin, M. Fairweather, X. Jia, R.A. Williams, University of Leeds/UK

3.47   **Study of non-linear dynamics in reactive distillation for TAME synthesis using equilibrium and non-equilibrium models**
A.M. Katariya, R.S. Kamath, S.M. Mahajani, K.M. Moudgalya, Indian Institute of Technology-Bombay, Mumbai/IND

3.48   **Simulation of (electro)chromatography by means of CFD**
D.-U. Astrath, Friedrich-Alexander-University Erlangen-Nuremberg/D; T. Schneider, Technische Universität Berlin/D; W. Arlt, Friedrich-Alexander-University Erlangen-Nuremberg/D

3.49   **Prediction and estimation techniques for modeling pervaporation process**
M.E.T. Alvarez, E.B. Moraes, M.R. Wolf-Maciel, State University of Campinas/BR

3.50   **ReDrop - an efficient simulation tool for describing solvent and reactive extraction columns**
M. Altunok, T. Grömping, A. Pfennig, RWTH Aachen/D

3.51   **Classical models of secondary settlers revisited**
R. David, A. Vande Wouwer, P. Saucez, Faculté Polytechnique de Mons/B; J.-L. Vasel, Université de Liège, Arlon/B

Biosystems modelling
3.52   **Mathematical modelling of three-dimensional cell cultures in perfusion bioreactors - part II**
F. Coletti, S. Macchietto, Imperial College London/UK; N. Elvassore, Università di Padova/I

3.53   **Metabolic regulatory network optimization using an information guided genetic algorithm approach**
Y. Zheng, Huazhong University of Science and Technology, Wuhan/PRC; C.-D. Yang, J.-W. Yeh, <u>S.-S. Jang</u>, M.F. Wu, Tsing-Hua University, Hsin-Chu/RC

3.54   **Minimal reaction sets and metabolic pathways for cultured hepatocytes**
H. Yang, M.L. Yarmush, C. Roth, <u>M.G. Ierapetritou</u>, Rutgers University, Piscataway, NJ/USA

3.55   **Hybrid modular mechanistic/ANN modelling of a wastewater phosphorous removal process**
<u>J. Peres</u>, Universidade do Porto/P; F. Freitas, M.A.M. Reis, Universidade Nova de Lisboa/P; S. Feyo de Azevedo, Universidade do Porto/P; R. Oliveira, Universidade Nova de Lisboa/P

3.56   **Modelling morphological change in endothelial cells induced by shear stress**
<u>R. Allen</u>, D.L. Bogle, A. Ridley, University College London/UK