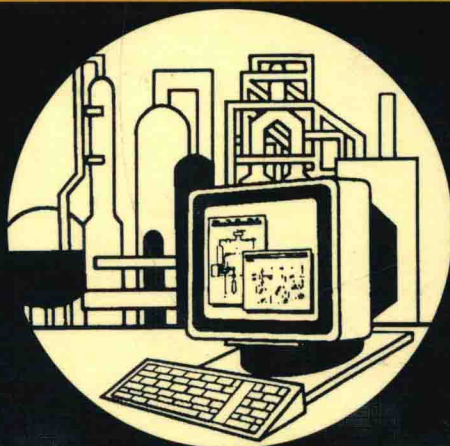


EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING - 10

Edited by
SAURO PIERUCCI



COMPUTER-AIDED CHEMICAL ENGINEERING, 8

ELSEVIER

EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING-10

33rd European Symposium of the Working Party on Computer Aided
Process Engineering

619th Event of the European Federation of Chemical Engineering (EFCE)

Organized by AIDIC, the Italian Association of Chemical Engineering

ESCAPE-10, 7-10 May, 2000, Florence, Italy

Edited by

Sauro Pierucci

*CIIC, Politecnico di Milano,
Piazza L. da Vinci, 32,
I-20133 Milan, Italy*



2000

Elsevier

Amsterdam – Lausanne – New York – Oxford – Shannon – Singapore – Tokyo

ELSEVIER SCIENCE B.V.
Sara Burgerhartstraat 25
P.O. Box 211, 1000 AE Amsterdam, The Netherlands

© 2000 Elsevier Science B.V. All rights reserved.

This work is protected under copyright by Elsevier Science, and the following terms and conditions apply to its use:

Photocopying

Single photocopies of single chapters may be made for personal use as allowed by national copyright laws. Permission of the Publisher and payment of a fee is required for all other photocopying, including multiple or systematic copying, copying for advertising or promotional purposes, resale, and all forms of document delivery. Special rates are available for educational institutions that wish to make photocopies for non-profit educational classroom use.

Permissions may be sought directly from Elsevier Science Rights & Permissions Department, PO Box 800, Oxford OX5 1DX, UK; phone: (+44) 1865 843830, fax: (+44) 1865 853333, e-mail: permissions@elsevier.co.uk. You may also contact Rights & Permissions directly through Elsevier's home page (<http://www.elsevier.nl>), selecting first 'Customer Support', then 'General Information', then 'Permissions Query Form'.

In the USA, users may clear permissions and make payments through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA; phone: (978) 7508400, fax: (978) 7504744, and in the UK through the Copyright Licensing Agency Rapid Clearance Service (CLARCS), 90 Tottenham Court Road, London W1P 0LP, UK; phone: (+44) 171 631 5555; fax: (+44) 171 631 5500. Other countries may have a local reprographic rights agency for payments.

Derivative Works

Tables of contents may be reproduced for internal circulation, but permission of Elsevier Science is required for external resale or distribution of such material.

Permission of the Publisher is required for all other derivative works, including compilations and translations.

Electronic Storage or Usage

Permission of the Publisher is required to store or use electronically any material contained in this work, including any chapter or part of a chapter.

Except as outlined above, no part of this work may be reproduced, stored in a retrieval system or transmitted in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, without prior written permission of the Publisher.

Address permissions requests to: Elsevier Science Rights & Permissions Department, at the mail, fax and e-mail addresses noted above.

Notice

No responsibility is assumed by the Publisher for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained in the material herein. Because of rapid advances in the medical sciences, in particular, independent verification of diagnoses and drug dosages should be made.

First edition 2000

Library of Congress Cataloging in Publication Data

A catalog record from the Library of Congress has been applied for.

ISBN: 0-444-50520-2

© The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

Printed in The Netherlands.

**EUROPEAN SYMPOSIUM ON
COMPUTER AIDED PROCESS
ENGINEERING - 10**

COMPUTER-AIDED CHEMICAL ENGINEERING

Advisory Editor: L.M. Rose

- Volume 1: Distillation Design in Practice (L.M. Rose)
- Volume 2: The Art of Chemical Process Design (G.L. Wells and L.M. Rose)
- Volume 3: Computer-Programming Examples for Chemical Engineers (G. Ross)
- Volume 4: Analysis and Synthesis of Chemical Process Systems (K. Hartmann and K. Kaplick)
- Volume 5: Studies in Computer-Aided Modelling, Design and Operation
 - Part A: Unit Operations (I. Pallai and Z. Fonyó, Editors)
 - Part B: Systems (I. Pallai and G.E. Veress, Editors)
- Volume 6: Neural Networks for Chemical Engineers (A.B. Bulsari, Editor)
- Volume 7: Material and Energy Balancing in the Process Industries - From Microscopic Balances to Large Plants (V.V. Veverka and F. Madron)
- Volume 8: European Symposium on Computer Aided Process Engineering-10 (S. Pierucci, Editor)

PREFACE

This book includes papers presented at ESCAPE10, the 10th European Symposium on Computer Aided Process Engineering, held in Florence, Italy, from the 7th to the 10th May, 2000.

ESCAPE10 was the tenth event of a series, started in Elsinore Denmark in 1992, of annual Symposia promoted by the Working Party 'Computer Aided Process Engineering (CAPE)' established in 1966 by the 'European Federation of Chemical Engineering (EFCE)'. However, it must be acknowledged that the ESCAPE series emerged from a strong tradition of the Working Party dating back to 1968 when the first event on computer applications was organized in Tutzing, Germany. Twenty three such symposia were then organized in almost a dozen European countries before a new departure of the Working Party with the ESCAPE series.

Therefore, ESCAPE-10 was the 33rd event of the CAPE Working Party, and the 609th event of the EFCE. The most recent symposia were organized in Hungary, Budapest 1999 (ESCAPE-9), Bruges, Belgium 1998 (ESCAPE-8), Trondheim, Norway 1997 (ESCAPE-7) and in Rhodes, Greece 1996 (ESCAPE-6). ESCAPE-10 was organized by AIDIC, the Italian Association of Chemical Engineering, a member society of the European Federation of Chemical Engineering.

The ESCAPE-10 scientific program reflected two complementary strategic objectives of the CAPE Working Party: the former checked the status of historically consolidated topics by means of their industrial application and their emerging issues, while the latter was addressed to opening new windows to the CAPE audience by inviting adjacent Working Parties to co-operate in the creation of the technical program.

The former CAPE strategic objective was covered by the topics:

Numerical Methods, Process Design and Synthesis, Dynamics & Control, Process Modeling, Simulation and Optimization.

The latter CAPE strategic objective derived from the EFCE promotion of scientific activities which autonomously and transversely work across the Working Parties terms of references. These activities should enhance the exchange of the know-how and knowledge acquired by different Working Parties in homologous fields. They also aim to discover complementary facets useful to the dissemination of WP's tools and of their novel procedures.

As a consequence the WP's 'Environmental Protection', 'Loss Prevention and Safety Promotion' and 'Multiphase Fluid Flow' were invited to assist in the organization of sessions in the area of:

***A Process Integrated approach for:
Environmental Benefit, Loss Prevention and Safety, Computational Fluid Dynamics.***

A total of 473 abstracts from all over the World were evaluated by the International Scientific Committee. Out of them 197 have been finally selected for the presentation and reported into this book. Their Authors come from 30 different Countries. The Selection of the papers was carried out by 28 international reviewers.

We hope that these proceedings will be a reference document to the scientific and industrial community and will contribute to the progress in Computer Aided Process Engineering.

Sauro Pierucci
Guido Buzzi Ferraris

SCIENTIFIC COMMITTEE

PIERUCCI Sauro	(Italy) co-Chairman
BUZZI FERRARIS Guido	(Italy) co-Chairman
AZZOPARDI Barry	(England)
BISTOLFI Marco	(Italy)
BOGLE David	(England)
BRIDGES Steven	(Denmark)
DONATI Gianni	(Italy)
ESPUNA Antonio	(Spain)
FRAGA Eric	(England)
GANI Rafiqul	(Denmark)
GLAVIC Peter	(Slovenia)
GREGERSEN Lars	(Denmark)
HEYEN George	(Belgium)
JORGENSEN John B.	(Denmark)
JOULIA Xavier	(France)
KRAVANJA Zdravko	(Slovenia)
Le LANN Jan Marc	(France)
MACCHIETTO Sandro	(England)
MEYER Michel	(France)
MEYER Xuan-Mi	(France)
PASMAN Hans J.	(The Netherlands)
PASTORINO Renato	(Italy)
PERRIS Tony	(England)
PUIGJANER-CORBELLA Luis	(Spain)
ROVAGLIO Maurizio	(Italy)
VENSELAAR Jan	(The Netherlands)
ZANELLI Severino	(Italy)
ZULLO Luca	(U.S.A.)

ORGANIZING COMMITTEE

Del ROSSO Renato	(Italy) Chairman
BALLO Giuliana	(Italy) Secretary
BENINCORI Carlo	(Italy)
POLI Giulio	(Italy)
WOLF MACIEL Maria Regina	(Brasil)

SYMPOSIUM SECRETARIAT

ESCAPE10 c/o AIDIC
Piazzale Morandi 2
I-20100 Milano (Italy)
Tel. +39-02-76021175
Fax +39-02-799644
e-mail: escape10@aidic.it
web : <http://www.aidic.it/escape-10/escape10.html>

VENUE

Palazzo Congressi, Florence, Italy
May 7-10, 2000

CONTENTS

Mixed Integer Non-Linear Programming Using Cutting Plane Techniques <i>R. Pörn and T. Westerlund</i>	1
A Novel Interactive MINLP Solver for CAPE Applications <i>J.P. Henriksen, S.F. Stoy, B.M. Russel and R. Gani</i>	7
An MILP-Based Reordering Algorithm for Complex Industrial Scheduling and Rescheduling <i>J. Roslöf, I. Harjunkoski, J. Björkqvist, S. Karlsson and T. Westerlund</i>	13
Non-Linear Partial Least Squares through Data Transformations <i>B. Li, E.B. Martin and A.J. Morris</i>	19
Optimisation of an Industrial Cogeneration System by means of a Multi-Objective Genetic Algorithm <i>G.A. Efthimeros, D.I. Pothianos, I.G. Katsipou, Z.G. Diamantis and D.T. Tsahalis</i>	25
Grid refinement in multiscale dynamic optimization <i>T. Binder, L. Blank, W. Dahmen and W. Marquardt</i>	31
Numerical Strategies for Optimal Experimental Design for Parameter Identification of Non-Linear Dynamic (Bio-)Chemical Processes <i>J.R. Banga, K.J. Versyck and J.F. Van Impe</i>	37
Solution of population balance equations for prediction of particle size distribution in emulsion polymerization: comparison and evaluation of different numerical methods <i>A.H. Alexopoulos and C. Kiparissides</i>	43
Solution of the hyperbolic model for heat and mass transfer in packed bed reactors <i>A.A. Iordanidi, A.E. Kronberg, J.A.M. Kuipers and K.R. Westerterp</i>	49
Moving finite difference method for tracking a shock or steep moving front <i>Y.I. Lim, S.H. Jeong, J.M. Le Lann and X. Joulia</i>	55
Neural Network in Physical Equilibria Prediction <i>S. Oreški, J. Zupan and P. Glavič</i>	61
Novel Methods for the Efficient Evaluation of Stored Mathematical Expressions on Vector Computers <i>B.R. Keeping and C.C. Pantelides</i>	67
Global Optimization of Nonconvex Problems with Differential-Algebraic Constraints <i>W.R. Esposito and C.A. Floudas</i>	73
Scheduling to Minimize Expected Completion Time in Flowshop Plants with Uncertain Processing Times <i>J. Balasubramanian and I.E. Grossmann</i>	79

Automatic Re-Weighting of Maximum Likelihood Functions for Parameter Regression	
<i>Y. Xin, V.R. Vasquez and W.B. Whiting</i>	85
Energy cost minimization in an energy intensive industrial plant: an MINLP approach	
<i>J. Vin, M.G. Ierapetritou, P. Sweeney and M. Chigirinskiy</i>	91
Generic object-oriented modelling, simulation and optimization of dynamical systems	
<i>T. Wack, G. Deerberg and S. Schlüter</i>	97
Detecting outliers in multivariate process data by using convex hulls	
<i>J.P. Barnard and C. Aldrich</i>	103
MINLP Optimization of Several Process Structures for the Separation of Azeotropic Ternary Mixtures	
<i>D. Brusis, T. Frey, J. Stichlmair, I. Wagner, R. Duessel and F.-F. Kuppinger</i>	109
MINLP Optimization of Reactive Distillation Columns	
<i>T. Frey and J. Stichlmair</i>	115
Batch Distillation Optimization with a Multiple Time-Scale Sequential Approach for Strong Nonlinear Processes	
<i>M. Wendt, P. Li and G. Wozny</i>	121
Non-Linear Constrained GRG Optimization under Parallel-Distributed Computing Environments	
<i>G.E. Vazquez, R. Rainoldi and N.B. Brignole</i>	127
A Bi-Index Continuous Time MILP Model for Short-Term Scheduling of Single-Stage Multi-Product Batch Plants with Parallel Units	
<i>C.-W. Hui and A. Gupta</i>	133
Importance of parameter selection in classification systems using neural networks	
<i>J. Ordieres and F. Ortega</i>	139
A two dimensional conceptual model to support data integration in process plant operations	
<i>A.D. Yang, H.-S. Li and M.-L. Lu</i>	145
Feedforward Control Based on Online Concentration Calculation of a Heat- and Mass-Integrated Distillation System	
<i>K. Löwe and G. Wozny</i>	151
Analysis of Input-Output Controllability in Reactive Distillation Using the Element model	
<i>A.D. Estrada-Villagrana, I.D.L. Bogle, E.S. Fraga and R. Gani</i>	157
Hybrid Simulation of Continuous Discrete Systems	
<i>V. Bahl and A.A. Linninger</i>	163
Interaction between Design and Control of Heat-Integrated PFR	
<i>C.S. Bildea, A.C. Dimian and P.D. Iedema</i>	169

Optimal control of batch reactors using Generic Model Control (GMC) and Neural Network	
<i>N. Aziz, M.A. Hussain and I.M. Mujtaba</i>	175
Stability analysis of delayed chemical systems	
<i>L. Pellegrini, M. Ratto and M. Schanz</i>	181
Nonlinear model based control of optimal temperature profiles in polystyrene polymerization reactor	
<i>G. Özkan, S. Özen, S. Erdogan, H. Hapoglu and M. Alpbaz</i>	187
Experimental Verification and Optimisation of a Detailed Dynamic High Performance Liquid Chromatographic Column Model	
<i>H.K. Teoh, M. Turner, N. Titchener-Hooker and E. Sorensen</i>	193
Expert Control of DO in the Aerobic Reactor of an Activated Sludge Process	
<i>M. Galluzzo, R. Ducato, V. Bartolozzi and A. Picciotto</i>	199
Dynamic Behavior of a Counter-Current Fixed-Bed Reactor with Sustained Oscillations	
<i>M. Mangold, F. Klose and E.D. Gilles</i>	205
Use of Gap Metric for Model Selection in Multi-Model Based Control Design: An Experimental Case Study of pH Control	
<i>O. Galán, J. Romagnoli, Y. Arkun and A. Palazoglu</i>	211
Dynamic and Control of High Purity Heterogeneous Azeotropic Distillation Process	
<i>C.J.G. Vasconcelos and M.R. Wolf-Maciel</i>	217
Training a Recurrent Neural Network by the Extended Kalman Filter as an Identification Tool	
<i>R. Scheffer and R. Maciel Filho</i>	223
An Algorithm for Efficient Specification Analysis in Large-Scale Dynamic Process Simulation	
<i>J.R. Paloschi</i>	229
Adaptive Neural Network Model Based Nonlinear Predictive Control of a Fluid Catalytic Cracking Unit	
<i>Z. Nagy, S. Agachi and L. Bodizs</i>	235
Computer Design of a System of Predictive Control for a Continuous Process Purification of Bioproducts	
<i>A. Mattedi and R. Maciel Filho</i>	241
Knowledge Based Modular Networks for Process Modelling and Control	
<i>J. Peres, R. Oliveira and S. Feyo De Azevedo</i>	247
Computer aided and control of a rotary kiln incinerator	
<i>E.T.I. de Souza, R. Maciel Filho and E. Tomas</i>	253
The use of process dynamic simulation for learning to design digital controllers	
<i>M.S. Basualdo, J. Salcedo B and D. Ruiz</i>	259
Model Based Control of Batch Chromatography	
<i>G. Dünnebier and K.-U. Klatt</i>	265

Model Predictive Control of an Industrial Dryer <i>V.M. Cristea, M. Baldea and Ş.P. Agachi</i>	271
Approximate Dynamic Models Using Coarse Grid Parameter Relaxation <i>V.J. Law</i>	277
Analysis of different control possibilities for the Divided Wall Column: feedback diagonal and Dynamic Matrix Control <i>M. Serra, M. Perrier, A. Espuna and L. Puigjaner</i>	283
Control Strategies for Brine Electrolysis by Ion Exchange Membrane Cell Process <i>Ş.P. Agachi and Á. Imre-Lucaci</i>	289
A new methodology for the active control of the heat transfer in Autoclave technology <i>V. Antonucci, M. Giordano, S. Inserra and L. Nicolais</i>	295
Model Predictive Control: A Multi-Parametric Programming Approach <i>A. Bemporad, N.A. Bozinis, V. Dua, M. Morari and E.N. Pistikopoulos</i>	301
Flowsheet Simulation for the Steel Industry - Using Experiences from Chemical Engineering and Modern Software Approaches <i>H. Müller, T. Peuker and G. Wozny</i>	307
Some aspects of rate-based modelling and simulation of three-phase distillation columns <i>E. Eckert and T. Vaněk</i>	313
Modeling and Simulation Tools for Supercritical Fluid Processes <i>S. Diaz, S. Espinosa and E.A. Brignole</i>	319
A computer aided tool for heavy oil thermal cracking process simulation <i>R. Maciel Filho and M.F. Sugaya</i>	325
Natural Gas Fired Power Plants with CO ₂ -Capture – Process Integration for High Fuel-to-Electricity Conversion Efficiency <i>H.M. Kvamsdal, T. Andersen and O. Bolland</i>	331
Simulation of convective drying of multicomponent moisture in a computer code MultidryPAK <i>Z. Pakowski</i>	337
An Algorithm for Analysis of Eletrolytic Liquid-Liquid Extraction Process for Concentration of Organic Acids <i>R.T.P. Pinto, L. Lintomen, A.J.A. Meirelles and M.R. Wolf-Maciel</i>	343
Estimation of the heat released by chemical reactions: Application to control of a simulated batch reactor <i>F. Xaumier, M.-V. Le Lann, M. Cabassud and G. Casamatta</i>	349
Modelling and Simulation of Biotechnological Processes: BIOSIM – A Package suitable for Integration in Process Engineering Tools <i>U. Bergstedt, H.J. Körner, S. Kabasci and G. Deerberg</i>	355
Simulation and Optimisation of Atmospheric and Vacuum Distillations of a Lube Plant <i>F.G. Martins, M.A.N. Coelho, C.A.V. da Costa, M.A.S. Jerónimo,</i>	

<i>C. Martins and A.S. Braga</i>	361
A coalescence and breakup module for implementation in CFD-codes	
<i>L. Hagesaether, H.A. Jakobsen, K. Hjarbo and H.F. Svendsen</i>	367
Fluid Dynamics and Thermochemical Simulation of a Smelting Cyclone	
<i>M. Modigell and M. Weng</i>	373
Computational Fluid Dynamics Modelling of Multiphase Reactors	
<i>M. Bistolfi, N. Mancini and F. Podenzani</i>	379
Simulation of silica deposition in an Atmospheric Pressure Chemical Vapour Deposition reactor, using a modified CFD software	
<i>J.P. Nieto, B. Caussat, J.P. Couderc, C. Artufel, S. Coletti, L. Jeannerot and O. Simonin</i>	385
Validation of a CFD model of a novel recycle axial flow cyclone for droplets removal from gas streams	
<i>D. Stanbridge, R. Swanborn, C.P. Heijckers and Z. Olujic</i>	391
Simulating Flow and Heat Transfer in Tubes Using a Fast CFD Formulation	
<i>E.R.L. Mercado, V.C. Souza, R. Guirardello and J.R. Nunhez</i>	397
Improving the Flow of Stirred Vessels with Anchor Type Impellers	
<i>S. M. C. P. Pedrosa, C.G. Duarte and J.R. Nunhez</i>	403
Influence of turbulence modelling and grid discretization on the simulation of flow-forces on tubes in cross-flow	
<i>K. Schröder and H. Gelbe</i>	409
A CFD - Finite Volume Method to Generate Deterministic Model: Application to Stirred Tank Reactors	
<i>R. Maciel Filho and V.M.F. Bezerra</i>	415
Simulation of Nox formation of glass melting furnaces by an integrated computational approach: CFD+Reactor Network Analysis	
<i>D. Benedetto, M. Falcitelli, S. Pasini and L. Tognotti</i>	421
CFD-Analysis of Heat Transfer and Initiator Mixing Performance in LDPE High Pressure Tubular Reactors	
<i>F.O. Mähling, A. Daiß, N. Kolhapure and R.O. Fox</i>	427
Dynamic Simulation of Complex Reaction Schemes and Biochemical Applications in Stirred Tank Reactors with Respect to Imperfect Mixing	
<i>U. Boltersdorf, G. Deerberg and S. Schlüter</i>	433
The steady state analysis of the twin helix heat exchanger	
<i>E.D. Lavric and V. Lavric</i>	439
Simulation of the bubble formation dynamics in rheologically complex fluids	
<i>H.Z. Li and Y. Mouline</i>	445
Coarse-grained formulation for the time evolution of intermaterial contact area density in mixing systems	
<i>A. Adrover, M. Fidaleo and M. Giona</i>	451
Dynamic Optimization of Semicontinuous Emulsion Copolymerization Reactions: Composition and Molecular Weight Distribution	
<i>C. Sayer, G. Arzamendi, J.M. Asua, E.L. Lima and J.C. Pinto</i>	457

Optimizing the Operation of a Sequential-Simulated Moving-Bed Separation Process Using MINLP	
<i>S. Karlsson, F. Pettersson, H. Skrifvars and T. Westerlund</i>	463
Multiperiod Planning for a Utility System Considering Emergency Situation by New Approach	
<i>J.H. Kim, S. Ju, C. Han and S.H. You</i>	469
Minimization of Natural Gas and Water Consumption in the Operation of Utility Plants	
<i>S.M. Corvalán and A.M. Eliceche</i>	475
Dynamic optimization of chemical and biochemical processes using restricted second order information	
<i>E. Balsa-Canto, J.R. Banga, A.A. Alonso and V.S. Vassiliadis</i>	481
Interaction Between Process Plant Operation and Cracking Furnaces Maintenance Policy in an Ethylene Plant	
<i>E. Schulz, S. Diaz and A. Bandoni</i>	487
Convergence Refinement of Stochastic Optimization by Coupling a Genetic Algorithm and a Simulated Annealing Procedure	
<i>A. Davin, C. Azzaro-Pantel, P. Floquet, L. Pibouleau and S. Domenech</i>	493
Fuzzy Modeling of Catalytic Multi-phase Reactor	
<i>B.B. Freitas Jr. and R. Maciel Filho</i>	499
Strategy and Mathematical Development for Scale-Up of Molecular Distillators for Recovering Carotenoids from Palm Oil	
<i>C.B. Batistella, E.B. Moraes, M.R.W. Maciel and R. Maciel Filho</i>	505
Characterization and quantification of liquid distribution in a packed column on a pilot scale	
<i>M.S. Kobayasi, M.R. Wolf-Maciel, F.A.N. Fernandes, D. Moraes Jr. and S.M. Pizzo</i>	511
Sensitivity in Optimization of a Reactor System with Deactivating Catalyst	
<i>I. Lovik, M. Hillestad and T. Hertzberg</i>	517
Detailed Mathematical Modelling of Membrane Modules	
<i>J.I. Marriott, E. Sørensen and I.D.L. Bogle</i>	523
A novel approach to the analysis of distillation columns for multicomponent mixtures	
<i>A.R. Giona, M. Giona and L.L.M. Lombardi</i>	529
ROME: A Repository to Support the Integration of Models over the Lifecycle of Model-based Engineering Processes	
<i>L. Von Wedel and W. Marquardt</i>	535
Increase business benefits by using on-line models.	
<i>D. Dempf and T. List</i>	541
Symbolic Discretization of Population Models for Process Simulation	
<i>M. Brahmadata, R. Köhler, A. Mitrović, E.D. Gilles and M. Zeitz</i>	547

Heat Integration in Process Design and Retrofit – Software Tools and Data Interchange - <i>E. Aust, S. Scholl and C. Übler</i>	553
Modelling and optimisation of polymerisation reactors in gPROMS <i>M. Asteasuain, S.M. Tonelli, A. Brandolin and J.A. Bandoni</i>	559
Modeling Particle Size Distribution (PSD) in Emulsion Copolymerization Reactions in a Continuous Loop Reactor <i>P.H.H. Araújo, J.C. de la Cal, J.M. Asua and J.C. Pinto</i>	565
Process modelling of metallurgical processes – software tool and modelling concept <i>M. Modigell, A. Traebert, P. Monheim, S. Petersen and U. Pickartz</i>	571
Modelling High Pressure Extraction Processes <i>M. Škerget and Ž. Knez</i>	577
Waterless wool cleaning process with supercritical carbon dioxide: extractor modeling and optimisation <i>F. Trabelsi, J-C. Luc, J. Miquel, M-A. Larrayoz, M. Capilla and F. Recasens</i>	583
Equation Based SPYRO [®] Model and Solver for the Simulation of the Steam Cracking Process <i>M.W.M. van Goethem, F.I. Kleinendorst, C. van Leeuwen and N. van Velzen</i>	589
A Shortcut Method for Design and Synthesis of Multicomponent Thermally Coupled Distillation Flowsheets <i>B.G. Rong, A. Kraslawski and L. Nyström</i>	595
A heating-cooling management to improve controllability of batch reactor equipped with a mono-fluid heating-cooling system <i>H. Bouhenchir, M. Cabassud, M.V. Le Lann and G. Casamatta</i>	601
Evaluation of time varying parameters in polymerization reactors by means of Temperature Oscillation Calorimetry <i>P. Guerrini De Luca, C. Scali and G. Maschio</i>	607
Integer-Programming Based Algorithms and Computational Performance for Terminal-Drop Zone Assignment Problems <i>M-T. Kong and N. Shah</i>	613
Automatic Generation of Switching Start-Up Schemes for Chemical Processes <i>E. Klein, A. Itigin, J. Raisch and A. Kienle</i>	619
Creative Design of Distillation Flowsheets Based on Theory of Solving Inventive Problems <i>B.G. Rong, A. Kraslawski and L. Nyström</i>	625
Technological change by system design - the industrial production of aromatics <i>G.P.J. Dijkema and J. Grievink</i>	631
Symmetric multiprocessing algorithm for conceptual process design <i>E.S. Fraga</i>	637

Optimisation of distillation and pervaporation system for ethanol dehydration <i>Z. Sztikai, Z. Lelkes, E. Rev and Z. Fonyo</i>	643
Shape and Terminal Velocity of Single Bubble Motion: a Novel Approach <i>G. Bozzano and M. Dente</i>	649
The Myth of Decomposition <i>P. Kesavan and P.I. Barton</i>	655
Parameter Analysis and Optimization of Ideal Heat Integrated Distillation Columns (HIDiC) <i>M. Nakaiwa, K. Huang, K. Naito, A. Endo, M. Owa, T. Akiya, T. Nakane and T. Takamatsu</i>	661
Computer-aided screening of adsorbents and porous catalyst carriers <i>F. Štěpánek, M. Marek, M. Kubíček and P.M. Adler</i>	667
A Hierarchical Framework for Modelling Biopharmaceutical Manufacture to Address Process and Business Needs <i>S. Farid, J. Washbrook, J. Birch and N. Titchener-Hooker</i>	673
Study of the insertion of partial oxidation gas turbine to satisfy high temperature requirements of industrial processes using energy integration techniques <i>F. Marechal and B. Kalitventzeff</i>	679
Abstract design in the development of pharmaceutical processes <i>M. Sharif, N.J. Samsatli and N. Shah</i>	685
Batch Distillation of Azeotropic Mixtures in a Column with a Middle Vessel <i>M. Warter and J. Stichlmair</i>	691
Development and design of a forced unsteady-state reactor through numerical simulation <i>M. Cittadini, M. Vanni, A.A. Barresi and G. Baldi</i>	697
Intent and Rationale in the Design of Chemical Processes: A Case Study <i>A. Guzmán-Reyna and R. Bañares-Alcántara</i>	703
Energy Efficient Distillation by Optimal Distribution of Heating and Cooling Requirements <i>T.R. Andersen, G. Siragusa, B. Andresen, P. Salamon and S.B. Jorgensen</i>	709
Optimal Design of Heat-Integrated Multipurpose Batch Facilities <i>A.P.F.D. Barbosa-Póvoa, T. Pinto and A.Q. Novais</i>	715
Plant-independent Process Representation <i>K. Wall, P.N. Sharratt, N. Sadr-Kazemi and J.N. Borland</i>	721
The design and management of material cycles towards a functional specification for an awareness-tool <i>E.V. Verhoef, G.P.J. Dijkema and M.A. Reuter</i>	727
A Strategy for the Generation of Robust Accident Scenarios in Quantitative Risk Assessment Using Multi-Component Analysis <i>K.H. Kim, J.H. Song, D. Shin and E.S. Yoon</i>	733

Simulation of Blowout Events: Integration of Different Modelling Approaches Within Industrial Risk Assessment and Management Tools <i>N. Mancini, F. Podenzani, M. Bonuccelli, P. Andreussi, P. Blotto and R. Galinetto</i>	739
Fault diagnosis system support for reactive scheduling in multipurpose batch chemical plants <i>D. Ruiz, J. Cantón, J.M. Nougues, A. Espuña and L. Puigjaner</i>	745
Improving on chemical process safety through distributed computer assisted knowledge analysis of preliminary design <i>B.A. Schupp, S.M. Lemkowitz, L. Goossens, H.J. Pasman and A.R. Hale</i>	751
Plant Monitoring and Fault Detection: Synergy between Data Reconciliation and Principal Component Analysis <i>T. Amand, G. Heyen and B. Kalitventzeff</i>	757
Note on vapour disengagement dynamics modelling <i>A. Sogaro, M.L. Caldi, D. Franchi and G. Biardi</i>	763
Computer aided transportation risk assessment <i>R. Bubbico, S. Di Cave and B. Mazzarotta</i>	769
Using PHA Results for Real Time Operator Support during ASM <i>S. Dash and V. Venkatasubramanian</i>	775
Leak Detection and Localisation in Pipes and Pipelines <i>G. Geiger, W. Gregoritz and D. Matko</i>	781
Industrial Applications of Intelligent Systems for Operating Procedure Synthesis and Hazards Analysis for Batch Process Plants <i>J. Zhao, S. Viswanathan and V. Venkatasubramanian</i>	787
Model-based safety verification under uncertainty <i>H. Huang, C.S. Adjiman and N. Shah</i>	793
Computerized Screening of Chemicals for Energy Release Hazards <i>B.K. Harrison</i>	799
A Hybrid Modular Hierarchical Approach for Fault Diagnosis in Complex Transient Processes <i>N. Scenna, B. Drozdowicz, S.J. Benz and E.J. Lamas</i>	805
Dynamic Simulation of the Behaviour of Pressure Relief Systems <i>J-P. Pokki, J. Aittamaa and M. Hurme</i>	811
From Environmental Care to Sustainability: the role of CAPE tools and methods <i>J. Venselaar</i>	817
Accounting for sustainability requirements in process design <i>M.P.C. Weijnen, P.M. Herder and H.D. Goel</i>	823
An Intelligent System for Identifying Waste Minimization Opportunities in Chemical Processes <i>I. Halim and R. Srinivasan</i>	829

A CAPE tool for evaluation of adsorber-reactor systems for treatment of exhausts from mobile sources	
<i>J. Jirát, M. Kubíček and M. Marek</i>	835
Quick identification of the wastewater biological treatment process by using shortcut techniques and previous plant operation data	
<i>G. Maria, C. Constantinescu and P. Ozil</i>	841
Implementation of Flue Gas Cleaning Systems into an Object-Oriented Process Simulator for Practical Use	
<i>G. Schuster, K. Weigl and A. Friedl</i>	847
Dynamic optimisation of small size wastewater treatment plants including nitrification and denitrification processes	
<i>B. Chachuat, N. Roche and M.A. Latifi</i>	853
A New Procedure for Predicting NO _x Emissions from Furnaces	
<i>T. Faravelli, L. Bua, A. Frassoldati, A. Antifora, L. Tognotti and E. Ranzi</i>	859
Liquid Effluent Properties Prediction from an Industrial Wastewater Treatment Plant Using Artificial Neural Networks	
<i>C.A. Gontarski, P.R. Rodrigues, M. Mori and L.F. Prenem</i>	865
Incorporating Production Scheduling in the Optimal Operation of Wastewater Treatment Plants	
<i>R. Gouveia and J.M. Pinto</i>	871
Analysis of the Operation of a NSDX Pilot Plant for Cr(VI) Recovery	
<i>A.M. Eliceche, S.M. Corvalán, A.I. Alonso and I. Ortiz</i>	877
Optimum deNO _x performance using inferential feedforward reductant flow control	
<i>H.C. Krijnsen, J.C.M. van Leeuwen, R. Bakker, H.P.A. Calis and C.M. van den Bleek</i>	883
Software tool for waste treatment selection using economic and ecological assessments	
<i>L. Cavin, O. Jankowitsch, U. Fischer and K. Hungerbühler</i>	889
Distributed Information System For Environmentally Conscious Process Design	
<i>Y. Fukushima and M. Hirao</i>	895
Decision Making for Batch Manufacturing Sites under Uncertainty	
<i>A.A. Linninger and A. Chakraborty</i>	901
Minimization of Water Consumption and Wastewater Discharge in the Sugar Cane Industry	
<i>R. Pastor, L. Abreu, A. Espuña and L. Puigjaner</i>	907
Hydrodynamics and Chemical Model to Evaluate Environmental Risks in Proximity of River Mouth	
<i>M. Di Natale, G. Merola and D. Musmarra</i>	913
Simulation and optimization of the reactive absorption of HF/HNO ₃ during pickling acid regeneration	
<i>W. Wukovits, W. Karner, A. Lebl, M. Harasek and A. Friedl</i>	919