F. Keil
W. Mackens
H. Voß
J. Werther
Editors

Scientific Computing in Chemical Engineering II

Computational Fluid Dynamics, Reaction Engineering, and Molecular Properties

$$i\epsilon\,\partial_t\Psi = \left(-\frac{\epsilon^2}{2}\Delta_q - \frac{1}{2}\Delta_x + V(x,q)\right)\Psi.$$

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Scientific Computing in Chemical Engineering II

Computational Fluid Dynamics, Reaction Engineering, and Molecular Properties

With 189 Figures and 29 Tables

Springer

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Preface

The present proceedings assemble the contributions to the second workshop on "Scientific Computing in Chemical Engineering". The two volumed edition covers the wide spectrum of computational activities in chemical process engineering encompassing tasks from process development, process design and optimization to process operations and control. The increasing performance of computers and the rapid advancement of numerical techniques encourages the employment of more sophisticated models. Quantum chemical approaches, molecular dynamics and Monte Carlo methods penetrate engineering design of catalysts and the calculation of phase transfer phenomena. Computational fluid dynamics of multi-phase flow is now a standard tool in chemical plant design. Numerical simulations replace time consuming and, therefore, expensive experiments to an ever increasing extent. The present workshop reflects these developments.

The large number of contributions made it necessary to split the proceedings into two volumes. We grouped the contributions into ten sections with the headings *Simulation of Reactive Flows, Reaction Engineering, Reaction Diffusion Problems, Molecular Properties, Computer Aided Process Design, Combustion and Flame, Image Processing, Optimization, Control* and *Neural Networks.* The present volume deals with the first four of them including the invited presentations related to these topics. The companion volume deals with the remaining six.

The workshop was organized by the Collaborative Research Center (Sonderforschungsbereich) 238 of the Deutsche Forschungsgemeinschaft "In-situ measuring techniques and dynamic modelling of multiphase flow systems" at the Technical University of Hamburg-Harburg in cooperation with the German Society for Chemical Apparatus, Chemical Engineering and Biotechnology e.V. (DECHEMA), the special interest groups "Scientific Computing" and "Industrial Mathematics" of the Deutsche Mathematiker Vereinigung (DMV), the joint special interest group "Numerical Software" of the DMV, the Gesellschaft für Angewandte Mathematik und Mechanik (GAMM), and the Gesellschaft für Informatik (GI), as well as the GAMM special interest group "Scientific Computing".

We thank all the people from these societies and groups who helped to realize both these proceedings and the workshop. We are grateful to our large number of referees for their careful inspection of the contributed papers and their valuable comments which increased the quality of the proceedings considerably.

Last but not least it is a pleasure for us to thank Dipl.-Phys. Ing. Vera Lochmann and Margitta Janssen for their untiring efforts in collecting all contributions and adapting them to the Springer LaTeX conventions.

The Editors

Contents

Preface V

1 Invited Presentations 1

Molecular Simulation: Phase Equilibria and Confined Systems 2
Keith E. Gubbins

Efficient Bifurcation Analysis of Forced Periodic Processes ... 12
Dan Luss, Johannes Khinast

Mathematical Modeling of the Coupling of Chemical Kinetics With Flow and Molecular Transport 26
Ulrich Maas

Non-Adiabatic Effects in Quantum-Classical Molecular Dynamics 42
Christof Schütte, Peter Nettesheim

2 Molecular Properties 57

Molecular Dynamics Simulation of Penetrant Transport in Organic/Inorganic Composite Membrane Materials 58
Martin Böhning, Dieter Hofmann, Dieter Paul

ParaGauss: A Density Functional Approach to Quantum Chemistry on Parallel Computers..... 66
Th. Belling, Th. Grauschopf, S. Krüger, F. Nörtemann, M. Staufer, M. Mayer, V. A. Nasluzov, U. Birkenheuer, N. Rösch

Mathematics for Combinatorial Chemistry..... 74
Th. Grüner, A. Kerber, R. Laue M. Meringer

Monte Carlo Simulation of Diffusion within Three-dimensional Pores with Irregular Walls 82
Xiang-yun Guo Frerich J. Keil

Molecular Modeling of Polymers..... 90
Reinhard Hentschke Thomas Flebbe, Ewald Aydt

Extension of Modified UNIFAC to Refrigerant Mixtures..... 98
Michael Kleiber, Joachim K. Axmann

Simulation of Transport and Diffusion on the Voronoi Network 106
V.A. Luchnikov, N.N. Medvedev, V.P. Voloshin, A. Geiger

Monte Carlo Modeling of Surface Diffusion in Interacting Systems with Phase Transitions 114
F. Nieto, A.A. Tarasenko, C. Uebing

Hydrophobic Aggregation of Nonionic Surfactants in Aqueous Solution: An MD Simulation Study 126
Dietmar Paschek, Thomas Engels, Wolfgang v. Rybinski, Alfons Geiger

Molecular Dynamics Simulations of Polymer-Membrane/Solvent Interfaces 134
Claudia Schepers, Dieter Hofmann, Dieter Paul

3 Reaction Diffusion Problems 143

A Continuation Framework for Invariant Subspaces and Its Application to Traveling Waves 144
Wolf-Jürgen Beyn, Winfried Kleß, Vera Thümmler

Sensitivity Analysis of Multicomponent Mass Transport in Porous Solids Described by Partial Differential Equations .. 152
Pavel Čapek, Andreas Seidel-Morgenstern

Simulation of the Diffusant Distribution in the Diffuse Furnace with Wafers 160
Orest Korbetsky, Victoria Kotchubey

Modelling and Simulation of Transient Transport Processes Using Axial Dispersion Model 167
Xing Luo, Bernd Niemeyer

A New Sparse Matrix Storage Method for Adaptive Solving of Reaction-Diffusion-Transport Equations 175
Nicolas Neuss

The Numerical Simulation of Annular Chromatography by Adaptive Finite Element Method 183
A. Thiele, L. Tobiska

4 Reaction Engineering 191

Modeling of Thermal Degradation of Polymers 192
Henning Bockhorn, Andreas Hornung, Ursel Hornung, Petra Jakobström, Michael Wulkow

Influence of Occupancy and Pore Network Topology on Tracer and Transport Diffusion in Zeolites 200
Marc-Olivier Coppens, Alexis T. Bell, Arup K. Chakraborty

Modeling of Pressure Fields in Fluids in Various Environments Including Damping Effects and Change of Wave Velocity Due to the Emergence of Cavitation Bubbles 208
Sascha Dähnke, Frerich J. Keil

On the Solution of Nonlinear Fractional-Order Differential Equations Used in the Modeling of Viscoplasticity 217
Kai Diethelm, Alan D. Freed

Stability Analysis of Chemical Reactors 225
M. A. Efendiev, A. Schuppert

Simulation of the Non-Stationary Behaviour of Fixed-Bed Reactors for the Determination of Kinetic Expressions in Consideration of Inhomegeneous Concentration Profiles Inside the Catalyst Pellets 231
Abdul Garayhi, Frerich Keil

A Dynamic Model for the Venturi Loop Reactor 239
Robbert de Graaf, Remco Reinstra, Maurits Wieberdink, Michiel Kreutzer

Numerical Modelling of Multiphase–Multicomponent Systems in Porous Media 247
R. Huber, R. Helmig

Efficient Computation of Singularities of Chemical Reactor Models 255
Johannes Khinast, Dan Luss

Computational Numerical Approaches in the Simulation of SMB Process 263
Celina P. Leão, Diana Azevêdo, Alírio E. Rodrigues

A Two Dimensional Population Model for a Continuous Crystallizer 271
A. Mitrović, S. Motz, A. Gerstlauer, C. Gahn, E.-D. Gilles

PE - a Scientific Computer Program for the Calculation of Fluid-Phase Equilibria 279
Oliver Pfohl, Stanimir Petkov, Gerd Brunner

Solving Chemical Engineering Problems with Front Propagation Using an Adaptive Moving Grid Method 287
A. Salden, J. Frauhammer, G. Eigenberger

Dynamic Simulation of Reactive Absorption Processes for the Purification of Coke Oven Gases 295
R. Schneider, E.Y. Kenig A. Górak

Remarks on the Numerical Treatment of Polymerization Processes 303
Peter Seifert

Direct Determination of Cyclic Steady States of Cyclically Operated Packed Bed Reactors 311
T.L. van Noorden, S.M. Verduyn Lunel, A. Bliek

5 Simulation of Reactive Flows 319

On Error Control for Reactive Flow Problems 320
Roland Becker, Malte Braack, Rolf Rannacher

Numerical Simulation of a Silicon Floating Zone with a Free Capillary Surface 328
Eberhard Bänsch, Burkhard Höhn

Prediction of Pressure Losses in Porous Media Using the Lattice Boltzmann Method 336
Jörg Bernsdorf, Francis Delhopital, Gunther Brenner, Franz Durst

Simulation and Analysis of Mixing in Two-Dimensional Turbulent Flows Using Fourier and Wavelet Techniques 344
Henning Bockhorn, Wolfgang Gerlinger, Kai Schneider, Jörg Ziuber

Direct Numerical Simulation of Marangoni Convection in a Twofluid System 352
Thomas Boeck, André Thess

Computation of Flows with Free Surfaces 360
Ismet Demirdzić, Samir Muzaferija, Milovan Perić, Eberhard Schreck, Volker Seidl

Simulation of Reactive Flow in a Partial Oxidation Reactor with Detailed Gas Phase and Surface Chemistry Models 368
Olaf Deutschmann, Lanny D. Schmidt, Jürgen Warnatz

Generalized Multiresolution Analysis on Unstructured Grids 376
Oliver Friedrich , Friederike Schröder-Pander, Thomas Sonar

Computational Fluid Dynamics Applied to Chemical Reaction Engineering 383
J.A.M. Kuipers, W.P.M. van Swaaij

CFD Simulation Tool for the Systematic Examination of Effects on Band Spreading in Large Radial Columns 391
M. Lisso, G. Wozny, Y. Beste, W. Arlt

On Projection-Based Time-Splitting Schemes for Computing Chemically Reacting Flows 401
Andreas Prohl

Chemical Partial Equilibrium Model in Gasdynamics Problems 409
Vladimir I. Sakharov, Elena Fateeva

Modelling Transient Irradiation Intensities of Pool Flames 417
Steffen Staus, Axel Schönbucher

Index 425

Index of Complementary Volume 431

Author's Index 437

Author's Index of Complementary Volume ... 441

Contents of Complementary Volume

1 Invited Presentations 1

Direct Multiple Shooting Methods for Control and Optimization of DAE in Chemical Engineering 2
Irene Bauer, H. Georg Bock, Daniel B. Leineweber, Johannes P. Schlöder

Topology Based Comparison Technique for Vector Fields Using Earth Mover's Distance 19
Rajesh Batra, Yingmei Lavin, Lambertus Hesselink

New Algorithms for Nonlinear Generalized Disjunctive Programming 31
Ignacio E. Grossmann, Sangbum Lee

A Framework for Control, State Estimation, Fault Detection, and Verification of Hybrid Systems 46
Manfred Morari, Alberto Bemporad, Domenico Mignone

Optimisation of Hybrid Dynamic Processes 62
Constantinos C. Pantelides, Marios P. Avraam, Nilay Shah

Multi-Scale Approaches in Engineering and Scientific Computing 77
George Stephanopoulos

2 Combustion and Flame 93

Numerical Simulation of Soot Particle Size Distributions with a Discrete Galerkin Method 94
Jörg Appel, Henning Bockhorn, Michael Wulkow

Direct Numerical Simulation of 3d Flame Balls 102
Henning Bockhorn, Jochen Fröhlich, Wolfgang Gerlinger, Kai Schneider

Hybrid Mixed Discretization Methods for Combustion Problems in Porous Media 110
Peter Knabner, Gerhard Summ

Soot and NOx Formation in a Stationary Turbulent Combustor 118
Markus Kraft, Michael Balthasar, Fabian Mauss

A DNS Study of Curvature Effects in Turbulent Premixed Flames 126
Marc Lange, Jürgen Warnatz

3D-Modeling of Coal Combustion in Circulating Fluidized Beds 134
K. Luecke, T. Knoebig, J. Werther

Transient Modeling of a Catalytic Combustor: A Critical Review of Assumptions Commonly Made 142
Roland Wanker, Harald Raupenstrauch, Gernot Staudinger

3 Computer Aided Process Design 151

Parallel Modular Dynamic Process Simulation 152
Jürgen Borchardt, Klaus Ehrhardt, Friedrich Grund, Dietmar Horn

Parallel Solution of Reaction-Diffusion Equations with a Stabilization Method 160
Uwe Kleis

Integration of Membrane Technology in Process Synthesis - Exemplary Separation of Acetic Acid - Water 168
G. Krabbe, R. Günther, J. Hapke, H. Kadereit, G. Schembecker

Hahn Polynomials and the Efficient Modelling of Fractionation 176
Peter Lory

Coupling Iterative Subsystem Solvers 184
Wolfgang Mackens, Jürgen Menck, Heinrich Voss

Work Control for Newton Type Coupling 192
Jürgen Menck

The Use of Numerical Tracking of Homoclinic and Heteroclinic Orbits in the Analysis of Chemical Engineering Problems 200
Igor Schreiber, Martin Kohout, Milan Kubíček

Modelling and Numerical Simulation of a Crosscurrent Heat Exchanger 208
Yvonne Wagner

4 Control 217

Efficient Direct Multiple Shooting in Nonlinear Model Predictive Control 218
Hans Georg Bock, Moritz Diehl, Daniel Leineweber, Johannes Schlöder

Control Concepts for Parabolic Equations with an Application to the Control of Fluid Flow 228
Michael Hinze, Andreas Kauffmann

Iterative Learning Control of Fluidized Bed Combustor for Sewage Sludge 236
Jan Lunze, Andreas Wolff

Numerical Solution of Variable Coefficient DAEs and Descriptor System 244
Peter Kunkel, Volker Mehrmann, Werner Rath

5 Image Processing 253

A Non Linear Diffusion Approach to Investigate Flow Structures in Circulating Fluidized Bed Reactors 254
Ariane Bredebusch, Klaus Wiehler, Hans Burkhardt, Rolf-R. Grigat

Flow Visualization with Textures 262
Thomas Loser, Dieter Mewes, Yuval Levy, Lambertus Hesselink

4-D Particle Tracking Velocimetry Applied to Gas-Liquid Reactors 270
Michael Stöhr, Christoph Garbe, Dirk Engelmann, Peter Geißler, Susana Gomes, Frank Hering, Bernd Jähne, Hans-Günter Wagner

6 Optimization 281

Numerical Methods for Initial Value Problems and Derivative Generation for DAE Models with Application to Optimum Experimental Design of Chemical Processes 282
Irene Bauer, Hans Georg Bock, Stefan Körkel, Johannes P. Schlöder

Parameter Estimation for Nonlinear Transport and Degradation Processes of Xenobiotica in Soil 290
Angelika E. Dieses, Johannes P. Schlöder, Hans Georg Bock, Otto Richter

Combined Stochastic and Gradient-Based Optimization 298
A. R. J. Esparta, E. Stein, A. Spieker, E. D. Gilles

A Scalable Discrete Optimization Algorithm for Heat Integration in Early Design 306
Eric S. Fraga, Ken I. M. McKinnon

Simulated Annealing for the Optimization of Chemical Batch Production Processes 314
Michael Hanke, Klaus R. Schneider

Convex Relaxations for Global Constrained Optimization Problems 322
Christian Jansson

The Concept of Contiguity in Models Based on Time-Indexed Formulations 330
Josef Kallrath

A Sequential Approach for Nonlinear Optimum Experimental Design in DAE Systems 338
Stefan Körkel, Irene Bauer, Hans Georg Bock, Johannes P. Schlöder

Application of Direct Search Optimization for Parameter Estimation 346
Rein Luus

Process Optimization of Reactive Systems Modeled by Elementary Reactions 354
Volker Schulz, Olaf Deutschmann

Dynamic Optimization of Multicomponent Distillation Processes 362
Erik Stein, Achim Kienle, Ernst D. Gilles

7 Neural Network 371

Trajectory Tracking of a Batch Polymerization Reactor Based on Input–Output–Linearization of a Neural Process Model ... 372
Joachim Horn

Early Detection and Identification of Undesirable States in Chemical Plants Using Neural Networks 380
Joachim Neumann, Görge Deerberg, Stefan Schlüter, Wilfried Schmitt, Günther Hessel

Adaptation of Dynamic Process Models with Integral Data A Lagrangian Approach 388
Josef Wagenhuber

Part I

Invited Presentations