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Nota di contenuto	Modeling of Process Intensification; Contents; Preface; List of Contributors; 1 Modeling of Process Intensification - An Introduction and Overview; 2 Process Intensification - An Industrial Point of View; 2.1 Introduction; 2.1.1 Remarks on the Term Process Intensification; 2.1.2 Management Aspects; 2.2 Microreaction Technology; 2.2.1 Principal Features; 2.2.2 Catalytic Wall Reactors; 2.3 Simulation; 2.3.1 Introduction; 2.3.2 Molecular Simulations; 2.3.2.1 Quantum-chemical Calculations; 2.3.2.2 COSMO-RS Calculations; 2.3.2.3 Molecular-dynamics Calculations 2.3.3 Monte Carlo Simulations in Project Valuation under Risk3 Modeling and Simulation of Microreactors; 3.1 Introduction; 3.2 Flow Distributions; 3.2.1 Straight Microchannels; 3.2.2 Periodic and Curved Channel Geometries; 3.2.3 Multichannel Flow Domains; 3.3 Heat

Transfer; 3.3.1 Straight Microchannels; 3.3.2 Periodic and Curved Channel Geometries; 3.3.3 Multichannel Flow Domains; 3.3.4 Micro Heat Exchangers; 3.4 Mass Transfer and Mixing; 3.4.1 Simple Mixing Channels; 3.4.2 Chaotic Micromixers; 3.4.3 Multilamination Micromixers; 3.4.4 Hydrodynamic Dispersion; 3.5 Chemical Kinetics 3.5.1 Numerical Methods for Reacting Flows 3.5.2 Reacting Channel Flows; 3.5.3 Heat-exchanger Reactors; 3.6 Conclusions and Outlook; 4 Modeling and Simulation of Unsteady-state-operated Trickle-flow Reactors; 4.1 Introduction; 4.2 Modeling; 4.3 Reactor Model; 4.4 Simulation; 4.5 Conclusion; 5 Packed-bed Membrane Reactors; 5.1 Introduction; 5.1.1 The PBMR Principle; 5.1.2 Case Study; 5.1.3 Porous Membranes; 5.1.4 Outline; 5.2 One-dimensional Modeling of Packed-bed Membrane Reactors; 5.2.1 One-dimensional Pseudohomogeneous Model 5.2.2 Cofeed (FBR) vs. Distributed Dosing of Reactants (PBMR) - Nonreactive Conditions 5.2.3 Comparison between FBR and PBMR - Reactive Conditions; 5.2.4 Nonisothermal Operation; 5.3 Two-dimensional Modeling of Packed-bed Membrane Reactors; 5.3.1 Two-dimensional Model of PBMR - The Momentum-balance Equation; 5.3.2 Two-dimensional Model of PBMR - The Mass-balance Equation; 5.3.3 Two-dimensional Model of PBMR - The Energy-balance Equation; 5.3.4 Boundary Conditions; 5.3.5 Numerical Solution of the Two-dimensional Model; 5.3.6 Velocity Field in a Packed-bed Membrane Reactor 5.3.7 The Influence of Membrane Permeability on the Boundary Conditions 5.3.8 Effect of Porosity Profile; 5.3.9 Effect of Radial Mass-transport Limitations; 5.3.10 Comparison of the (r)- and (w)-model Concepts - Temperature Profiles in a PBMR; 5.4 Three-dimensional Modeling of a Packed-bed Membrane Reactor; 5.4.1 Introduction to the Large-scale Simulation Methods in Fluid Mechanics and Mass Transport; 5.4.2 Pressure and Velocity Field (Varying the Flow Distribution) - Comparison between FBR and PBMR; 5.4.3 Advective-diffusive Mass Transport in PBMR; 5.5 Summary and Conclusion 6 The Focused Action of Surface Tension versus the Brute Force of Turbulence - Scaleable Microchannel-based Process Intensification using Monoliths

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#### Sommario/riassunto

Combining the knowledge involved in process engineering and process modeling, this is the first book to cover all modeling methods applicable to process intensification. Both the editors and authors are renowned experts from industry and academia in the various fields of process modeling and integrated chemical processes. Following an introduction to the topic, the book goes on to look at equipment and operational methods, monolithic catalysis, HEX, micro- and reverse flow reactors, catalytic and reactive distillation, the simulated-moving bed and vibration bubble column as well as ultraso

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