

CONTENTS

CONTRIBUTORS.	ix
PREFACE	xi

A Review of Multiscale Analysis: Examples from Systems Biology, Materials Engineering, and Other Fluid–Surface Interacting Systems

DIONISIOS G. VLACHOS

I. Introduction	2
II. Deterministic, Continuum Models	6
A. Hierarchy of Models.	7
B. Solving Deterministic, Continuum Differential Equation Models: Techniques and Status.	8
III. Overview of Discrete, Particle Models.	8
A. Hierarchy of Stochastic Models for Well-mixed, Chemically Reacting Systems	9
B. Solving Master Equations Stochastically: Monte Carlo Methods.	10
IV. Classification of Multiscale Simulation Approaches	12
V. Hybrid Multiscale Simulation.	14
A. Onion-type Hybrid Multiscale Simulations and Algorithms	15
B. Application of Onion-type Hybrid Multiscale Simulation to Growth of Materials.	17
C. Applications of Onion-type Hybrid Multiscale Simulation to Other Areas	23
D. Multigrid-type Hybrid Multiscale Simulations	24
E. An Example of Multigrid-type Hybrid Multiscale Simulation for Growth under Large Length Scale Gradients	26
F. Challenges in Hybrid Multiscale Simulations	28
VI. Coarse Graining of Stochastic Models	32
A. Temporal Upscaling of KMC Simulation in Well-mixed Systems.	32
B. Spatial Upscaling of Distributed (Lattice) KMC Simulation.	36
C. Spatiotemporal Acceleration of Distributed (Lattice) KMC Simulation	38
VII. Multiscale, Stochastic Modeling of Biological Networks.	40
A. Spatially Well-mixed Systems	40
B. Spatially Distributed Systems	44
VIII. Systems Tasks	45
A. Sensitivity and Identifiability Analyses.	46
B. Parameter Estimation from Experimental Data and Finer Scale Models	51
C. Model Reduction and Control.	53
D. Bifurcation	54

IX. Outlook	55
Acknowledgments	55
References	56

Quantifying Physics and Chemistry at Multiple Length-scales using Magnetic Resonance Techniques

LYNN F. GLADDEN, MICHAEL D. MANTLE AND ANDREW J. SEDERMAN

I. Introduction	64
II. Principles of MR Measurements	68
A. Spatially Unresolved And Spatially Resolved Experiments.	69
B. Nuclear Spin Relaxation Times	73
C. Transport	76
D. Temperature.	83
E. The $\mathbf{k}$ -space Raster.	83
F. Fast Data Acquisition.	87
III. Recent Developments in MR as a Tool in Chemical Engineering Research.	92
A. “Ultra-fast” Imaging of Velocity Fields	93
B. Multiple Images From a Single Excitation	96
C. Imaging Rotating Systems	98
D. “Ultra-fast” Diffusion Measurement.	99
E. Gas-phase MR	100
IV. Reaction Engineering: From Catalyst to Reactor.	103
A. MR Spectroscopy of Catalysts.	103
B. Micro-imaging and Molecular Diffusion Studies of Formed Catalyst Pellets.	105
C. Single-Phase Flow in Fixed-Bed Reactors.	110
D. Measuring Chemical Composition and Mass Transfer in Fixed-Bed Reactors: In Situ Studies of Reactions	115
E. Two-Phase Flow in Fixed-Bed Reactors.	119
F. Hydrodynamic Transitions in Fixed-Bed Reactors.	123
V. Future Prospects.	128
Acknowledgments.	130
References	131

Modeling of transport and transformation processes in porous and multiphase bodies

JURAJ KOSEK, FRANTIŠEK ŠTĚPÁNEK AND MILOŠ MAREK

I. Introduction	138
II. Methodology.	140
A. Representation of Multiphase Media.	140
B. Structure Acquisition	142
C. Morphological Characterization.	143

D. Digital Reconstruction of Multiphase Media	145
E. Calculation of Effective Properties	151
F. Effective-scale Transport Models	159
III. Transformations.	160
A. Skeletonization	161
B. Phase Transitions	161
C. Chemically Reactive Systems.	170
IV. Applications	175
A. Multi-scale Reconstruction of a Catalyst Pellet.	175
B. Reconstruction of Closed-cell Polymer Foam Structure.	179
C. Polymer Particle Morphogenesis	182
D. Granulation and Dissolution.	189
E. Simulation of CO Oxidation on Reconstructed Catalytic Washcoat	192
V. Outlooks	195
A. Biological Systems	195
B. Materials Design	196
VI. Conclusions.	197
Acknowledgments.	198
References	198

Spatially Averaged Multi-Scale Models for Chemical Reactors

SAIKAT CHAKRABORTY AND VEMURI BALAKOTAIAH

I. Introduction	206
A. A Brief History of Chemical Reactor Models.	208
B. Multi-scale Nature of Homogeneous and Catalytic Reactors	211
C. Different Approaches to Multi-scale Averaging or Dimension Reduction.	214
II. Spatial Averaging of Convection–diffusion–reaction Models using the L–S Method	217
III. Spatially Averaged Models for Describing Dispersion Effects in Tubes and Packed Beds	221
A. A Hyperbolic-Averaged Model for Describing Dispersion Effects in Tubes/Capillaries.	222
B. Multi-mode Hyperbolic Averaged Models for Describing Dispersion Effects in Chromatographs	233
C. A Hyperbolic Model for Describing Dispersion Effects in Monoliths with Diffusion into the Solid Phase.	238
IV. Spatially Averaged Multi-mode (Multi-scale) Models for Homogeneous Reactors	239
A. Isothermal Tubular Reactors.	239
B. Loop and Recycle Reactors	248
C. Tank Reactors (CSTRs)	250
D. Non-isothermal Reactor Models	252
E. Multiple Reactions.	259
F. Examples Illustrating Use of Multi-mode Homogeneous Reactor Models.	260
V. Spatially Averaged Multi-Mode (Multi-Scale) Models for Catalytic Reactors.	273
A. Wall-catalyzed Reactions.	273
B. Coupled Homogeneous and Wall-catalyzed Reactions	277

C. Non-isothermal Reactor Models	278
D. Examples Illustrating Use of Multi-mode Catalytic Reactor Models.	279
VI. Accuracy, Convergence and Region of Validity of Multi-mode/Multi-scale Averaged Models	283
A. Accuracy.	283
B. Convergence.	284
C. Regularization of the Local Equation	288
VII. Summary, Conclusions, and Recommendations for Future Work	293
Acknowledgments.	294
References	296
INDEX.	299
CONTENTS OF VOLUMES IN THIS SERIAL	303