Contents

About the Editors *XIII*
List of Contributors *XV*
Preface *XIX*

1 Chemical Engineering Science and Green Chemistry – The Challenge of Sustainability *1*
Alexei A. Lapkin
1.1 Sustainability Challenge for the Chemical Industry *1*
1.2 From Green to Sustainable Chemistry *5*
1.3 Chemical Engineering Science for Sustainability *7*
1.4 Trends in Chemical Engineering Science *9*
1.5 Topics Covered in This Book *11*
Acknowledgment *13*
References *13*

Part One: Molecular Engineering of Materials, Reactions, and Processes *17*

2 Recent Advances in the Molecular Engineering of Solvents for Reactions *19*
Eirini Siougkrou, Amparo Galindo, and Claire S. Adjiman
2.1 Introduction *19*
2.2 Solvent Effects on Reactions *22*
2.3 Design or Selection of Solvents for Chemical Reactions *26*
2.3.1 Model-Based Screening Methods *27*
2.3.2 Generate-and-Test Methods *28*
2.3.3 Optimization-Based Methods *30*
2.3.4 Discussion *34*
2.4 A Case Study *35*
2.5 Conclusions *38*
Acknowledgments *38*
References *39*

3 Hierarchically Structured Pt and Non-Pt-Based Electrocatalysts for PEM Fuel Cells *47*
Panagiotis Trogadas and Marc-Olivier Coppens
3.1 Introduction *47*
3.2 Pure Hollow Pt Nanoparticles *49*
3.3 Hollow Pt Metal Alloys *51*
3.3.1 PtAu *52*
3.3.2 PtAg *53*
3.3.3 PtCo *56*
3.3.4 PtNi *58*
3.3.5 PtRu *59*
3.3.6 PtPd *61*
3.3.7 PtCu *62*
3.4 Non-Pt Alloy Nanostructures *63*
3.5 Conclusions and Outlook *64*
Acknowledgment *65*
References *65*

4 New Frontiers in Biocatalysis *73*
John M. Woodley and Nicholas J. Turner
4.1 Introduction *73*
4.2 Recent Advances in Biocatalysis *74*
4.3 Biocatalytic Retrosynthesis *75*
4.4 Process-Driven Protein Engineering *80*
4.5 Process Developments *83*
4.5.1 Continuous Processes *83*
4.5.2 Kinetic Analysis *84*
4.6 Future Perspectives *84*
References *85*

Part Two: Innovations in Design, Unit Operations, and Manufacturing *87*

5 Conceptual Process Design and Process Optimization *89*
Alexander Mitsos, Ung Lee, Sebastian Recker, and Mirko Skiborowski
5.1 Introduction *89*
5.2 Mathematical Background *89*
5.2.1 System of Nonlinear Equations *90*
5.2.2 Nonlinear Programming (NLP) *90*
5.2.3 Mixed Integer Programming *92*
5.3 Synthesis *93*
5.3.1 Reactor Networks *93*
5.3.2 Separation Systems *95*
5.3.3 Overall Flowsheets *97*
5.4 Superstructure-Based Techniques *101*

5.4.1 Heat Exchange Networks *101*
5.4.2 Process Flowsheet Optimization *103*
5.5 Integrated Process Design, Operation, and Control *105*
5.6 Water and Energy Processes *105*
5.7 Conclusions and Outlook *107*
References *107*

6 Development of Novel Multiphase Microreactors: Recent Developments and Future Challenges *115*
Evgeny Rebrov
6.1 Principles and Features *115*
6.1.1 Continuous Phase Multiphase Microreactors *115*
6.1.1.1 Falling Film Microreactor *115*
6.1.1.2 Mesh Contactor *116*
6.1.2 Dispersed Phase Multiphase Microreactors *116*
6.1.2.1 Segmented Flow Microreactors *116*
6.1.2.2 Microstructured Packed Beds *117*
6.1.2.3 Prestructured Microreactors *118*
6.1.2.4 Foam Microreactors *120*
6.1.2.5 Microreactors with Fibrous Internal Structures *120*
6.2 Experimental Practice *121*
6.2.1 Flow Regimes *121*
6.2.1.1 Capillary Microreactors *121*
6.2.1.2 Structured Packed Beds *122*
6.2.2 Dispersion and Holdup in Microstructured Packed Bed Reactors *123*
6.2.2.1 Liquid Holdup *123*
6.2.2.2 Hydrodynamic Dispersion *124*
6.3 Modeling Features *125*
6.3.1 Hydrodynamics *125*
6.3.1.1 Falling Films Microreactors *125*
6.3.2 Pressure Drop in Capillary Microreactors *127*
6.3.2.1 Gas–Liquid Microreactors *127*
6.3.2.2 Liquid–Liquid Microreactors *130*
6.3.3 Mass Transfer *131*
6.3.3.1 Capillary Microreactors *131*
6.3.3.2 Falling Film Microreactors *133*
6.3.4 Two-Phase Flow Distribution *133*
6.4 Applications *136*
6.4.1 Falling Film Microreactors *136*
6.4.2 Capillary Microreactors *137*
6.4.2.1 Wall Coated Catalytic Microreactors *137*
6.4.2.2 Phase Transfer Catalysis in Microreactors *139*
6.4.2.3 Microstructured Packed Bed Reactors *142*
6.5 Conclusions and Outlook *144*
References *144*

7 Process Intensification through Continuous Manufacturing: Implications for Unit Operation and Process Design *153*
Sebastian Falß, Nicolai Kloye, Manuel Holtkamp, Angelina Prokofyeva, Thomas Bieringer, and Norbert Kockmann
7.1 Continuous Processes as a Means of Process Intensification *153*
7.2 Equipment for Continuous Processes *158*
7.2.1 Upstream Equipment *159*
7.2.1.1 Reactors without Active Mixing *159*
7.2.1.2 Reactors with Dynamic Mixing *161*
7.2.2 Downstream Equipment *163*
7.2.3 Process Integration *165*
7.2.4 Continuous Equipment as Enabling Technology *166*
7.3 Process Development and Implementation for Continuous Processes *168*
7.3.1 Process Development and Scale-Up *168*
7.3.2 Flexible Implementation of Continuous Processes *172*
7.4 Selected Case Studies *174*
7.5 Conclusion and Outlook *180*
References *182*

8 How Technical Innovation in Manufacturing Is Fostered through Business Innovation *191*
Nicolas Eghbali, Marianne Hoppenbrouwers, Steven Lemain, Gert De Bruyn, and Bart Vander Velpen
8.1 General Introduction *191*
8.2 Concept of Chemical Leasing and Take Back Chemicals *192*
8.2.1 The Concept of Take Back Chemicals *194*
8.2.2 Advantages and Challenges of the Take Back Chemicals Model *195*
8.2.2.1 What Are the Advantages of Implementing TaBaChem *196*
8.2.2.2 What Are the Impediments in Implementing the New Business Models? *197*
8.3 General Economic, Technical, and Management Aspects *198*
8.3.1 Economic Aspects *198*
8.3.1.1 Direct Gains, Indirect Gains, and Investments *198*
8.3.1.2 Pricing *199*
8.3.1.3 Conclusion on the Economic Aspects *200*
8.3.2 Technical Aspects *201*
8.3.2.1 Reuse of Chemicals *201*
8.3.2.2 Process Optimization *201*
8.3.2.3 Conclusion on the Technical Aspects *201*
8.3.3 Organizational/Managerial Aspects *202*
8.3.3.1 Sales *202*
8.3.3.2 Quality Assurance *202*
8.3.3.3 Tendering and Rewarding *202*

8.3.3.4 Knowledge Sharing *202*
8.3.3.5 Logistics *203*
8.3.3.6 Conclusion on the Organizational/Managerial Aspects *203*
8.4 Compatibility of the Service Model with the Actual Legislation: Some Important Aspects *203*
8.4.1 Transition from Sales to Providing a Service to the Customer *204*
8.4.1.1 The Supplier Retains Ownership of the Chemical *204*
8.4.1.2 Result-Oriented Services Lead to Different Pricing of a Chemical *204*
8.4.1.3 A Transparent and Elaborated Contract Is Necessary *205*
8.4.2 Closing the Life Cycle and Preventing Waste *205*
8.4.3 Business Confidentiality and the Protection of Competition *208*
8.4.3.1 Intellectual Property Rights *208*
8.4.3.2 Competition *208*
8.5 General Conclusion *211*
References *211*

9 Applications of 3D Printing in Synthetic Process and Analytical Chemistry *215*
Victor Sans, Vincenza Dragone, and Leroy Cronin
9.1 Introduction *215*
9.1.1 Polymerization-Based Additive Manufacturing (AM) *216*
9.1.1.1 Stereolithography (SLA) *217*
9.1.1.2 Photopolymer Jetting (PJ) *217*
9.1.1.3 Physical Binding *217*
9.1.2 Melting-Based Techniques *218*
9.1.2.1 Selective Laser Melting (SLM) *218*
9.1.2.2 Electron Beam Melting (EBM) *218*
9.1.2.3 Fused Deposition Modeling (FDM) *219*
9.1.2.4 Laser Sintering (LS) *219*
9.1.2.5 Material Jetting (MJ) *219*
9.2 Chemical Reactors Manufacturing by Additive Manufacturing Techniques *220*
9.2.1 3D Printing Technologies in Chemistry *220*
9.3 3D Printing Applied to Flow Chemistry *226*
9.3.1 Mesoscale Reactors *226*
9.3.2 3D Printed Membranes *235*
9.4 Applications of 3D Printed Flow Devices in Analytical Chemistry *239*
9.4.1 3D Printing of Valves, Pumps and Actuators *239*
9.4.2 Modular Devices Based on SL *242*
9.5 Future Trends *248*
9.5.1 Ultrafast Printing *249*
9.5.2 Smart Materials through 4D Printing *250*

9.6 Conclusions *251*
References *252*

Part Three: Enabling Technologies *257*

10 Process Analytical Chemistry and Nondestructive Analytical Methods: The Green Chemistry Approach for Reaction Monitoring, Control, and Analysis *259*
Miriam Fontalvo Gómez, Boris Johnson Restrepo, Torsten Stelzer, and Rodolfo J. Romañach
10.1 Green Chemistry and Chemical Analysis in Manufacturing *259*
10.2 Process Analytical Chemistry: Concept and Objectives *260*
10.3 Vibrational Spectroscopy *264*
10.4 Challenges to Overcome *268*
10.5 Applications of Process Analytical Chemistry and Nondestructive Analyses *270*
10.5.1 Dairy Industry *270*
10.5.2 Synthesis of Active Pharmaceutical Ingredients *271*
10.5.3 Preparation of Polymeric Strip Film Unit Dosage Forms *273*
10.5.4 Polymer Industry *274*
10.5.5 Process Analytical Chemistry for Biodiesel Production *276*
10.6 Future Trends in PAC *279*
Acknowledgments *281*
References *281*

11 NMR Spectroscopy and Microscopy in Reaction Engineering and Catalysis *289*
Carmine D'Agostino, Mick D. Mantle, and Andrew J. Sederman
11.1 Introduction *289*
11.2 Basic Principles of NMR *290*
11.2.1 Nuclear Spins and Bulk Magnetization *290*
11.2.2 NMR Spectroscopy of Liquids *293*
11.2.3 NMR Relaxation *295*
11.2.3.1 Spin–Lattice Relaxation *295*
11.2.3.2 Spin–Spin Relaxation *296*
11.2.4 Pulsed Field Gradient NMR *297*
11.3 The NMR Toolkit in Reaction Engineering and Catalysis *299*
11.3.1 NMR Spectroscopy in Catalysis and Reaction Engineering *300*
11.3.2 Diffusion of Fluids Confined in Porous Catalysts *306*
11.3.2.1 Catalyst Deactivation Studies Using PFG NMR *311*
11.3.3 NMR Relaxation Time Analysis in Porous Catalytic Materials *314*
11.3.4 Combining NMR Spectroscopy with Magnetic Resonance Imaging *319*
11.4 Summary *324*
References *324*

12 An Introduction to Closed-Loop Process Optimization and Online Analysis *329*
Christopher S. Horbaczewskyj, Charlotte E. Willans, Alexei A. Lapkin, and Richard A. Bourne
12.1 Introduction *329*
12.2 Principles of Self-Optimization and Requirements for Experimental Systems *330*
12.3 Analytical Techniques for Closed-Loop Optimization *332*
12.4 Decision Algorithms in Closed-Loop Optimization *334*
12.4.1 Algorithms for Discovery *335*
12.4.2 Algorithms for Developing Process Understanding *337*
12.4.3 Algorithms for Automated Process Optimization *338*
12.5 Application Examples of Closed-Loop Discovery and Optimization *341*
12.5.1 Discovery in Closed-Loop Self-Optimization *341*
12.5.2 High-Throughput Screening *342*
12.5.3 Examples of One-Variable-at-a-Time Reaction Optimization *344*
12.5.4 Examples of Application of Design of Experiments *346*
12.5.5 Rate-Based/Physical Organic Approaches *350*
12.5.6 Examples of Algorithm-Based Self-Optimization *364*
12.6 Conclusions and Future Directions *368*
Acknowledgments *369*
References *369*

Index *375*