

# **Catalysis for the Conversion of Biomass and Its Derivatives**

Malte Behrens and Abhaya K. Datye

**Edition Open Access  
2013**

# Contents

	<b>Introduction</b> .....	1
	Opening Remarks .....	1
	List of Authors, Communicator and Editors .....	6
<b>1</b>	<b>Raw Material Change in the Chemical Industry and the Role of Biomass</b>	
	<i>Friedrich Seitz</i> .....	15
1.1	Introduction .....	15
1.2	Raw Material Alternatives .....	15
1.3	Existing Businesses with Renewables .....	17
1.4	Existing Businesses with Renewables: Issues .....	18
1.5	The Use of Biomass .....	19
1.6	Outlook/Conclusions .....	20
1.7	Figures .....	23
<b>2</b>	<b>The Role of Startup Companies in the Conversion of Biomass to Renewable Fuels and Chemicals</b>	
	<i>Leo E. Manzer</i> .....	43
2.1	Introduction .....	43
2.2	Results and Discussion .....	44
2.3	Conclusion .....	57
<b>3</b>	<b>Nutrient Cycling in the Bioeconomy: A Life Cycle Perspective</b>	
	<i>Robert Anex</i> .....	61
3.1	Introduction .....	61
3.2	Life Cycle Assessment Methodology .....	62
3.3	Life Cycle Inventory .....	65
3.4	Impact Assessment .....	67
3.5	LCA of Biorenewable Chemical Systems .....	68
3.6	Prospective, Consequential, and Attributional LCA .....	71
3.7	Resource Constraints on Biorenewable Chemical Production .....	72
3.8	Conclusion .....	76

<b>4</b>	<b>Plant Growth: Basic Principles and Issues Relating to the Optimization of Biomass Production and Composition as a Feedstock for Energy</b>	
	<i>Mark Stitt</i> .....	83
4.1	Introduction: The Contribution of Plants to the Global Carbon Cycle .....	83
4.2	Is the Glass Half Full or Half Empty? .....	87
4.3	Low Energy Conversion Efficiency in Photosynthesis .....	90
4.4	The Use of Photosynthesis to Drive Plant Growth .....	103
4.5	Vegetative Biomass: What to Do with the Cell Walls? .....	109
4.6	Response of Photosynthesis and Plant Growth to Rising Atmospheric Carbon Dioxide .....	112
4.7	Integrated Model of Energy Use Efficiency during Photosynthesis and Growth .....	113
4.8	What is Needed for Efficient Energy Crops? .....	116
4.9	Current Energy Crops and Their Shortcomings .....	116
<b>5</b>	<b>Biomass Chemistry</b>	
	<i>Michael Ladisch, Eduardo Ximenes, Youngmi Kim, Nathan S. Mosier</i> .....	131
5.1	Introduction .....	131
5.2	Feedstock Availability .....	131
5.3	The Role of Petroleum .....	133
5.4	The Cost of Biomass Feedstocks .....	134
5.5	Maximum Yield as a Function of Biomass Composition .....	136
5.6	Location .....	139
5.7	Metrics for Biochemical vs. Thermochemical Conversion .....	140
5.8	Biomass Chemistry .....	142
5.9	Hydrolysis of Polysaccharides in Cellulosic Biomass .....	147
5.10	Chemistry of Pretreatment .....	148
5.11	Chemical Degradation and Inhibitor Formation During Pretreatment .....	149
5.12	Impact of Formed Inhibitors .....	153
5.13	Conclusions .....	158
<b>6</b>	<b>Chemical and Biological Deconstruction of Aqueous Phase Processing</b>	
	<i>Charles E. Wyman, Carol J. Wyman</i> .....	165
6.1	Introduction .....	165
6.2	Why Cellulosic Biomass? .....	166

6.3	Conversion Options for Aqueous Phase Processing . . . . .	168
6.4	Laboratory Methods to Make Reactive Intermediates . . . . .	171
6.5	Pretreatments and Biological Production of Sugars as Reactive Intermediates Through the Consortium for Applied Fundamentals and Innovation (CAFI) . . . . .	172
6.6	Thermochemical Processing to Sugars and Other Reactive Intermediates . . . . .	177
6.7	Conclusions . . . . .	178
<b>7</b>	<b>Analytical Approaches in the Catalytic Transformation of Biomass: What Needs to be Analyzed and Why?</b> <i>Dmitry Murzin, Bjarne Holmbom</i> . . . . .	183
7.1	Introduction . . . . .	183
7.2	Analytical Objectives . . . . .	185
7.3	Basic Analytical Methods . . . . .	186
7.4	Analytical Examples . . . . .	195
7.5	Final Words . . . . .	206
<b>8</b>	<b>Methods for Biomass Compositional Analysis</b> <i>Amie Sluiter, Justin Sluiter, Edward J. Wolfrum</i> . . . . .	213
8.1	Introduction . . . . .	213
8.2	Biomass Composition . . . . .	214
8.3	Measuring Biomass Composition: Forage and Fiber Analysis . . . . .	215
8.4	Summative Compositional Analysis of Biomass Feedstocks . . . . .	217
8.5	Summative Compositional Analysis of Pretreated Biomass Slurries and Liquors . . . . .	228
8.6	Summative Mass Closure-Calculations, Troubleshooting, and Errors . . . . .	233
8.7	Uncertainty in the Primary Measurements . . . . .	235
8.8	Propagation of Uncertainty in Primary Measurements . . . . .	237
8.9	Room for Improvement in Biomass Compositional Analysis . . . . .	243
8.10	Rapid Biomass Analysis via NIR . . . . .	246
8.11	Conclusions . . . . .	247
	Appendix . . . . .	251
<b>9</b>	<b>Reaction Engineering Concepts for the Catalytic Conversion of Biorenewable Molecules</b> <i>Robert J. Davis</i> . . . . .	255
9.1	Introduction . . . . .	255
9.2	Measurement of Reaction Rates . . . . .	256
9.3	Kinetics of Chemical Reactions . . . . .	258

9.4	Deactivation of Catalysts .....	262
9.5	Reactors Used to Evaluate Catalysts .....	269
9.6	Mass and Heat Transfer Artifacts .....	270
9.7	Influence of Reactor Configuration .....	282
9.8	Conclusions .....	286
<b>10</b>	<b>Catalytic Strategies and Chemistries Involved in the Conversion of Sugars to Liquid Transportation Fuels</b>	
	<i>Elif I. Gürbüz, James A. Dumesic</i> .....	293
10.1	Introduction .....	293
10.2	Thermodynamic Considerations .....	293
10.3	Formulating Strategies for the Conversion of Sugars to Alkane Fuels: Platform Molecules .....	300
10.4	The Conversion of Sugars and Polyols to H <sub>2</sub> and Alkanes .....	309
10.5	Conversion of Sugars/Polyols to Liquid Fuels via the Formation of Monofunctional Intermediates .....	329
10.6	Levulinic Acid and $\gamma$ -Valerolactone Platforms for the Production of Liquid Fuels .....	337
10.7	Concluding Remarks .....	346
<b>11</b>	<b>Design of Heterogeneous Catalysts for the Conversion of Biorenewable Feedstocks</b>	
	<i>Brent H. Shanks</i> .....	361
11.1	Introduction .....	361
11.2	Adsorption of Carbohydrates and Their Derivatives on Solid Surfaces .....	364
11.3	Selective Bond Cleavage .....	371
11.4	Aqueous Phase Considerations .....	378
11.5	Novel Catalytic Materials for Biomass Conversion .....	384
11.6	Hydrothermally Stable Catalytic Materials .....	392
11.7	Impurity Tolerant Catalysts .....	396
11.8	Novel Reaction Systems .....	400
11.9	Summary .....	402
<b>12</b>	<b>Tailor-Made Fuels and Chemicals from Biomass</b>	
	<i>Thorsten vom Stein, Jürgen Klankermayer, Walter Leitner</i> .....	411
12.1	Introduction .....	411
12.2	Conceptual Approach to Tailor-Made Fuels via Combined Product and Process Design .....	412
12.3	From Intermediates to Products .....	414

12.4	From Lignocellulosic Raw Materials to Carbohydrate Feedstock and Platform Molecules .....	425
12.5	Conclusion and Outlook .....	428
<b>13</b>	<b>Solution-Based Deconstruction of (Ligno)-Cellulose</b>	
	<i>Roberto Rinaldi, Jennifer Reece</i> .....	435
13.1	Introduction .....	435
13.2	Understanding Cellulosic Recalcitrance .....	435
13.3	Cellulose in Solution .....	438
13.4	Homogeneous Hydrolysis of Cellulose .....	451
13.5	Final remarks .....	457