## **Contents**

1	CO <sub>2</sub> Capture – A Brief Review of Technologies and Its Integration 1
	Mónica García, Theo Chronopoulos, and Rubén M. Montañés
1.1	Introduction: The Role of Carbon Capture 1
1.2	CO <sub>2</sub> Capture Technologies 2
1.2.1	Status of CO <sub>2</sub> Capture Deployment 2
1.2.2	Pre-combustion 2
1.2.3	Oxyfuel 3
1.2.4	Post-combustion 3
1.2.4.1	Adsorption 4
1.2.4.2	High-Temperature Solids Looping Technologies 7
1.2.4.3	Membranes 8
1.2.4.4	Chemical Absorption 9
1.2.5	Others CO <sub>2</sub> Capture/Separation Technologies 13
1.2.5.1	Fuel Cells 13
1.3	Integration of Post-combustion CO <sub>2</sub> Capture in the Power Plant and
1.5	Electricity Grid 17
1.3.1	Integration of the Capture Unit in the Thermal Power Plant 17
1.3.2	Flexible Operation of Thermal Power Plants in Future Energy
1.5.2	Systems 20
1.4	CO <sub>2</sub> Capture in the Industrial Sector 21
1.5	Conclusions 22
1.5	References 24
	References 24
2	Advancing CCSU Technologies with Computational Fluid
	Dynamics (CFD): A Look at the Future by Linking CFD and
	Process Simulations 29
	Daniel Sebastia-Saez, Evgenia Mechleri, and Harvey Arellano-García
2.1	Sweep Across the General Simulation Techniques Available 29
2.2	Multi-scale Approach for CFD Simulation of Amine Scrubbers 32



vi	Contents
----	----------

4.2

2.3	Eulerian, Eulerian–Lagrangian, and Discrete Element Methods for the Simulation of Calcium Looping, Mineral Carbonation, and Adsorption in Other Solid Particulate Materials 38
2.4	CFD for Oxy-fuel Combustion Technologies: The Application of Single-Phase Reactive Flows and Particle Tracking Algorithms 41
2.5	CFD for Carbon Storage and Enhanced Oil Recovery (EOR): The Link Between Advanced Imaging Techniques and CFD 41
2.6	CFD for Carbon Utilization with Chemical Conversion: The Importance of Numerical Techniques on the Study of New Catalysts 44
2.7	CFD for Biological Utilization: Microalgae Cultivation 46
2.8	What Does the Future Hold? 47
	References 49
3	Membranes Technologies for Efficient CO <sub>2</sub>
	Capture - Conversion 55
	Sonia Remiro-Buenamañana, Laura Navarrete, Julio Garcia-Fayos, Sara
	Escorihuela, Sonia Escolastico, and José M. Serra
3.1	Introduction 55
3.2	Polymer Membranes 56
3.3	Oxygen Transport Membranes for CO <sub>2</sub> Valorization 60
3.3.1	Oxygen Transport Membrane Fundamentals 61
3.3.2	Application Concepts of OTMs for Carbon Capture and Storage (CCS) 63
3.3.3	Existing Developments 63
3.4	Protonic Membranes 65
3.4.1	Proton Defects in Oxide Ceramics 65
3.4.2	Proton Transport Membrane Fundamentals 67
3.4.3	Application Concepts of Proton Conducting Membranes 68
3.5	Membranes for Electrochemical Applications 69
3.5.1	Electrolysis and Co-electrolysis Processes 69
3.5.1.1	Water Electrolysis 70
3.5.1.2	CO <sub>2</sub> Co-electrolysis 73
3.5.2	Synthesis Gas Chemistry 75
3.5.3	Other Applications 76
3.5.3.1	Methane Steam Reforming 76
3.5.3.2	Methane Dehydroaromatization 78
3.6	Conclusions and Final Remarks 78
	References 79
4	Computational Modeling of Carbon Dioxide Catalytic
	Conversion 85
	Javier Amaya Suárez, Elena R. Remesal, Jose J. Plata, Antonio M. Márquez,
	and Javier Fernández Sanz
4.1	Introduction 85

General Methods for Theoretical Catalysis Research 85

4.3	Characterizing the Catalyst and Its Interaction with CO <sub>2</sub> Using DFT Calculations 87
4.4	Microkinetic Modeling in Heterogeneous Catalysis 89
4.5	New Trends: High-Throughput Screening, Volcano Plots, and Machine Learning 92
4.5.1	High-Throughput Screening 92
4.5.2	Volcano Plots and Scaling Relations 93
4.5.3	DFT and Machine Learning 93
4.5.3.1	Machine-Learned Potentials 95
4.5.3.2	Descriptors to Predict Catalytic Properties 95
4.5.3.3	Future Challenges in HT-DFT Applied to Catalysis 96 References 97
5	An Overview of the Transition to a Carbon-Neutral Steel Industry 105
	Juan C. Navarro, Pablo Navarro, Oscar H. Laguna, Miguel A. Centeno, and José A. Odriozola
5.1	Introduction 105
5.2	Global Relevance of the Steel Industry 106
5.2.1	Features that Make Steel a Special Material 107
5.3	Current Trends in Emission Policies in the World's Leading Countries in Steel Industry 109
5.4	Transition to a Carbon-Neutral Production. A Big Challenge for the Steel Industry 110
5.4.1	Urea 113
5.4.2	Methanol and Formic Acid 114
5.4.3	Carbon Monoxide 114
5.4.4	Methane 114
5.5	CO <sub>2</sub> Methanation: An Interesting Opportunity for the Valorization of the Steel Industry Emissions 114
5.6	Relevant Projects Already Launched for the Valorization of the CO <sub>2</sub> Emitted by the Steel Industry 116
5.7	Concluding Remarks 119 References 120
6	Potential Processes for Simultaneous Biogas Upgrading and Carbon Dioxide Utilization 125
	Francisco M. Baena-Moreno, Mónica Rodríguez-Galán, Fernando Vega,
	Isabel Malico, and Benito Navarrete
6.1	Introduction 125
6.2	Overview of Biogas General Characteristics and Upgrading Technologies
	to Bio-methane Production 127
6.2.1	Biogas Composition and Applications 127
6.2.2	Biogas Upgrading Processes 127
6.2.2.1	Water Scrubbing 129

viii	Contents
------	----------

6.2.2.2	Pressure Swing Adsorption 129
6.2.2.3	Chemical Scrubbing 129
6.2.2.4	Organic Physical Scrubbing 129
6.2.2.5	Membrane Separation 129
6.2.2.6	Cryogenic Separation 130
6.3	CCU Main Technologies 131
6.3.1	Supercritical CO <sub>2</sub> as a Solvent 131
6.3.2	Chemicals from CO <sub>2</sub> 132
6.3.3	Mineral Carbonation 132
6.3.4	Fuels from CO <sub>2</sub> 133
6.3.5	Algae Production 133
6.3.6	Enhanced Oil Recovery (EOR) 133
6.4	Potential Processes for Biogas Upgrading and Carbon Utilization 133
6.4.1	Chemical Scrubbing Coupled with CCU 134
6.4.2	Membrane Separation Coupled with CCU 135
6.4.3	Cryogenic Separation Coupled with CCU 136
6.5	Conclusions 138
	References 139
_	
7	Biogas Sweetening Technologies 145
	Nikolaos D. Charisiou, Savvas L. Douvartzides, and Maria A. Goula
7.1	Introduction 145
7.2	Biogas Purification Technologies 146
7.2.1	Removal of Water Vapor $(H_2O_{(g)})$ 146
7.2.2	Removal of Hydrogen Sulfide (H <sub>2</sub> S) and Other Sulfur-Containing
	Compounds 148
7.2.2.1	In Situ Precipitation of H <sub>2</sub> S Through Air/Oxygen Injection 148
7.2.2.2	In Situ Precipitation of H <sub>2</sub> S Through Iron Chloride/Oxide Injection 148
7.2.2.3	Adsorption by Activated Carbon 149
7.2.2.4	Zeolite-Based Sieve (Molecular Sieve) 150
7.2.2.5	Water Scrubbing 150
7.2.2.6	Organic Solvent Scrubbing 151
7.2.2.7	Sodium Hydroxide Scrubbing 151
7.2.2.8	Chemical Adsorption via Iron Oxide or Hydroxide (Iron Sponge) 152
7.2.2.9	Biological Filters 152
7.2.3	Removal of Siloxanes 153
7.2.3.1	Organic Solvent Scrubbing 154
7.2.3.2	Adsorption on Activated Carbon, Molecular Sieves, and Silica Gel 154
7.2.3.3	Membrane Separation 155
7.2.3.4	Biological Filters 156
7.2.3.5	Cryogenic Condensation 156  Removed of Volatile Organic Compound (VOCs) 156
7.2.4	Removal of Volatile Organic Compound (VOCs) 156
7.2.5	Removal of Ammonia (NH <sub>3</sub> ) 156  Removal of Ouygon (O.) and Nitrogen (N.) 157
7.2.6	Removal of Oxygen (O <sub>2</sub> ) and Nitrogen (N <sub>2</sub> ) 157
7.3 7.3.1	Biogas Upgrading Technologies 157 Water Scrubbing 157

7.3.2	Organic Solvent Scrubbing 160
7.3.3	Chemical Scrubbing 160
7.3.4	Pressure Swing Adsorption 162
7.3.5	Polymeric Membranes 163
7.3.6	Cryogenic Treatment 165
7.4	Conclusions 166
	References 166
8	CO <sub>2</sub> Conversion to Value-Added Gas-Phase Products:
	Technology Overview and Catalysts Selection 175
	Qi Zhang, Laura Pastor-Pérez, Xiangping Zhang, Sai Gu, and Tomas R Reina
8.1	Chapter Overview 175
8.2	CO <sub>2</sub> Methanation 176
8.2.1	Background 176
8.2.2	Fundamentals 177
8.2.3	Catalysts 178
8.2.3.1	Ruthenium-Based Catalysts 178
8.2.3.2	Nickel-Based Catalysts 179
8.2.3.3	Rhodium and Palladium-Based Catalysts 182
8.3	RWGS Reaction 183
8.3.1	Background 183
8.3.2	Fundamentals 184
8.3.3	Catalysts 184
8.3.3.1	Noble Metal-Based Catalysts 185
8.3.3.2	Copper-Based Catalysts 185
8.3.3.3	Ceria-Based Support Catalysts 186
8.3.3.4	Carbide Support Catalysts 187
8.4	CO <sub>2</sub> Reforming Reactions 188
8.4.1	Background 188
8.4.2	Fundamentals 189
8.4.3	Catalysts 190
8.4.3.1	Noble Metal-Based Catalysts 190
8.4.3.2	Ni-Based Catalysts 191
8.4.3.3	Catalytic Supports 193
8.5	Conclusions and Final Remarks 195
	References 195
0	CO Italiantian Emphasis by Missachannal Parators 205
9	CO <sub>2</sub> Utilization Enabled by Microchannel Reactors 205  Luis F. Bobadilla, Lola Azancot, and José A. Odriozola
9.1	Introduction 205
9.2	Transport Phenomena and Heat Exchange in Microchannel Reactors 207
0.2.1	
9.2.1	Microfluidics and Mixing Flow 208
9.2.2	Heat Exchange and Temperature Control 210
9.3	Application of Microreactors in CO <sub>2</sub> Capture, Storage, and Utilization
	Processes 212

×	Contents	
	9.3.1	CO <sub>2</sub> Capture and Storage (CCS) 212
	9.3.2	CO <sub>2</sub> as a Feedstock for Producing Valuable Commodity Chemicals 214
	9.3.2.1	Methanation of Carbon Dioxide (Sabatier Reaction) 214
	9.3.2.2	CO <sub>2</sub> -to-Methanol and Dimethyl Ether (DME) Transformation 217
	9.3.2.3	CO <sub>2</sub> -to-Higher Hydrocarbons and Fuels 218
	9.3.2.4	Production of Cyclic Organic Carbonates 219
	9.4	Concluding Remarks and Future Perspectives 221 References 221
	10	Analysis of High-Pressure Conditions in CO <sub>2</sub> Hydrogenation Processes 227
		Andrea Álvarez Moreno, Esmeralda Portillo, and Oscar Hernando Laguna
	10.1	Introduction 227
	10.2	Thermodynamic Aspects 229
	10.2.1	Le Chatelier Principle as a Simple Way to Understand the Effect of Pressure in Chemical Reactions 230
	10.2.2	Equilibrium Composition Calculations of High-Pressure Gas Reactions
		Based on the Computerized Gibbs Energy Minimization 232
	10.3	Overview of Some Industrial Approaches Focused on the Production of
		Valuable Compounds form CO <sub>2</sub> Using a Carbon Capture and Utilization
		(CCU) Approach 234
	10.3.1	Industrial Production of Methanol 235
	10.3.2	Production of Methane 237
	10.4	Techno-Economic Considerations for the Methanol Production from a
	10.5	CCU Approach with the Use of High Pressure 238 Concluding Remarks 248
	10.5	References 248
	11	Sabatier-Based Direct Synthesis of Methane and Methanol Using CO <sub>2</sub> from Industrial Gas Mixtures 253
	11.1	K. Müller, J. Israel, F. Rachow, and D. Schmeißer  Overview 253
	11.2	Methane Synthesis of Gas Mixtures 255
	11.2.1	Thermodynamics of Methane Conversion 255
	11.2.2	Experimental Setup, General Definitions, and Catalysts 256
	11.2.3	Industrial Gas Mixtures 258
	11.3	Applications 260 APP-01: Combustion Plant Flue Gas 260
	11.3.1	
	11.3.2	APP-02: Coke Oven Gas (COG) 264
	11.3.3	APP-03: Saline Aquifer Back-Produced CO <sub>2</sub> 267
	11.3.4	APP-04: Biogenic CO <sub>2</sub> Sources 268

APP-05: Oxyfuel Operation in Gas Engines 269
APP-06: Reusage of CH<sub>4</sub> Product Gas Mixtures 270

Methanol Synthesis 274

Acknowledgments 277 References 277

11.3.5

11.3.6

11.4

12	Survey of Heterogeneous Catalysts for the CO <sub>2</sub> Reduction to CO via Reverse Water Gas Shift 281 Thomas Mathew, Simi Saju, and Shiju N. Raveendran
12.1	Introduction 281
12.2	RWGS Catalysts 281
12.2.1	Supported Metal Catalysts 282
12.2.1.1	
12.2.1.2	•
12.2.1.3	•
12.2.1.4	•
12.2.1.5	Pd- and Ir-Based Catalysts 289
12.2.1.6	Cu-Based Catalysts 290
12.2.1.7	Ni-Based Catalysts 295
12.2.1.7	Oxide Systems 298
12.2.3	Transition Metal Carbides 300
12.3	Mechanism of RWGS Reaction 306
12.3	References 307
13	Electrocatalytic Conversion of CO <sub>2</sub> to Syngas 317
	Manuel Antonio Díaz-Pérez, A. de Lucas Consuegra, and Juan Carlos
	Serrano-Ruiz
13.1	Introduction 317
13.2	Production of Syngas 319
13.3	Electroreduction of CO <sub>2</sub> /Water Mixtures to Syngas 320
13.3.1	Effect of Cell Configuration and Chemical Environment 321
13.3.2	Effect of the Cathode Composition and Structure 324
13.3.3	Effect of the Reaction Parameters 327
13.3.4	Electrochemical Promotion of Catalyst (EPOC) for CO <sub>2</sub>
	Hydrogenation 328
13.4	Conclusions 329
	Acknowledgments 330
	References 330
14	Recent Progress on Catalyst Development for CO <sub>2</sub> Conversion
	into Value-Added Chemicals by Photo- and
	Electroreduction 335
14.1	Luqman Atanda, Mohammad A. Wahab, and Jorge Beltramini
	Introduction 335
14.2	CO <sub>2</sub> Catalytic Conversion by Photoreduction 336
14.2.1	Principle of CO <sub>2</sub> Photothermal Reduction 337
14.2.2	Catalyst Development for CO <sub>2</sub> Photothermal Reduction 339
14.3	CO <sub>2</sub> Catalytic Conversion by Electroreduction 346
14.3.1 14.3.2	Principle of CO <sub>2</sub> Electrocatalytic Reduction 347
14.3.4	Catalysts Development for CO <sub>2</sub> Electroreduction 349  References 357

15	Yolk@Shell Materials for CO <sub>2</sub> Conversion: Chemical and Photochemical Applications 361 Cameron Alexander Hurd Price, Laura Pastor-Pérez, Tomas Ramirez-Reina,
	and Jian Liu
15.1	Overview 361
15.2	Key Benefits of Hierarchical Morphology 363
15.2.1	
15.3	Materials for Chemical CO <sub>2</sub> Recycling Reactions 366
15.3.1	CO <sub>2</sub> Utilization Reactions 366
15.3.2	Photochemical Reactions with CO <sub>2</sub> 368
15.3.2.1	Principles of Photocatalysis 368
15.3.2.2	Prominent Materials 369
15.3.2.3	Benefits of YS in Photocatalysis 369
15.4	Synthesis Techniques for CS/YS: A Brief Overview 372
15.4.1	Soft Templating Techniques 373
15.4.2	Hard Templating Techniques 374
15.4.2.1	Metal Oxide/Carbide Shells 375
15.5	Future Advancement 375
	References 376
16	Aliphatic Polycarbonates Derived from Epoxides and
	CO <sub>2</sub> 385
161	Sebastian Kernbichl and Bernhard Rieger
16.1	Introduction 385
16.2	Aliphatic Polycarbonates 386
16.2.1	Synthesis of the Monomers 386  Machanistic Agnesis of the Caralymentistic of Francisco and CO 387
16.2.2	Mechanistic Aspects of the Copolymerization of Epoxides and CO <sub>2</sub> 387  Thormal Stability and Possible Dogradation Pathways 380
16.2.3 16.2.4	Thermal Stability and Possible Degradation Pathways 389 Mechanical Properties 390
16.3	Catalyst Systems for the CO <sub>2</sub> /Epoxide Copolymerization 392
16.3.1	Heterogeneous Catalysts 393
16.3.2	Overview of the Homogeneous Catalytic Systems 393
16.3.3	Terpolymerization Pathways 398
16.3.4	Limonene Oxide: Recent Advances in Catalysis and Mechanism
10.5.1	Elucidation 399
16.4	Conclusion 402
2011	References 402
17	Metal-Organic Frameworks (MOFs) for CO <sub>2</sub> Cycloaddition
	Reactions 407
	Ignacio Campello, Antonio Sepúlveda-Escribano, and Enrique V.
	Ramos-Fernández
17.1	Introduction to MOF 407
17.2	MOFs as Catalysts 407
17.2.1	Active Sites in MOFs: Lewis Acid Sites 409

17.2.1.1	Historical Overview 409
17.2.1.2	Tunability of the Lewis Acid Sites 411
17.2.1.3	Active Sites in MOFs: Lewis Basic Sites 413
17.3	CO <sub>2</sub> Cycloadditions 414
17.3.1	Reaction Mechanism 414
17.3.2	CO <sub>2</sub> Cycloadditions Reactions Catalyzed by Lewis Acid MOFs 415
17.3.3	CO <sub>2</sub> Cycloaddition Reactions Catalyzed by Lewis Acid and Basic MOFs 416
17.3.4	Defective MOFs for CO <sub>2</sub> Cycloaddition Reactions 416
17.3.5	MOFs Having Functional Linkers for CO <sub>2</sub> Cycloaddition Reactions 419
17.3.3	Oxidative Carboxylation 420
17.4	References 420
	TOTOLOGO 120
18	Plasma-Assisted Conversion of CO <sub>2</sub> 429
	Kevin H. R. Rouwenhorst, Gerard J. van Rooij, and Leon Lefferts
18.1	Introduction 429
18.1.1	What Is a Plasma? 430
18.1.2	History 430
18.1.3	Electrification 431
18.1.4	Thermodynamics 431
18.1.5	Homogeneous Plasma Activation of CO <sub>2</sub> 432
18.1.6	Mechanisms 433
18.1.7	Plasma Reactors 435
18.1.8	Performance in Various Plasma Reactors 436
18.2	Plasma-catalytic CO <sub>2</sub> Conversion 437
18.2.1	Introduction 437
18.2.2	Mutual Influence of Plasma and Catalyst 439
18.2.3	Catalyst Development 440
18.2.4	Experimental Performance 442
18.2.4.1	CO <sub>2</sub> Dissociation 443
18.2.4.2	Dry Reforming of Methane 444
18.2.4.3	CO <sub>2</sub> Hydrogenation 446
18.2.4.4	Artificial Photosynthesis 447
18.3	Perspective 448
18.3.1	Models Describing Plasma Catalysis 448
18.3.2	Scale-Up and Process Considerations 449
18.4	Conclusion 450
	References 451

Index 463