

## Contents

Preface *xv*

- 1 Shale Gas as an Option for the Production of Chemicals and Challenges for Process Intensification 1**  
*Andrea P. Ortiz-Espinoza and Arturo Jiménez-Gutiérrez*
  - 1.1 Introduction 1
  - 1.2 Where Is It Found? 1
  - 1.3 Shale Gas Composition 3
  - 1.4 Shale Gas Effect on Natural Gas Prices 3
  - 1.5 Alternatives to Produce Chemicals from Shale Gas 4
  - 1.6 Synthesis Gas 4
  - 1.7 Methanol 5
  - 1.8 Ethylene 6
  - 1.9 Benzene 7
  - 1.10 Propylene 7
  - 1.11 Process Intensification Opportunities 8
  - 1.12 Potential Benefits and Tradeoffs Associated with Process Intensification 10
  - 1.13 Conclusions 11
  - References 11
  
- 2 Design and Techno-Economic Analysis of Separation Units to Handle Feedstock Variability in Shale Gas Treatment 15**  
*Eric Bohac, Debalina Sengupta, and Mahmoud M. El-Halwagi*
  - 2.1 Introduction 15
  - 2.2 Problem Statement 16
  - 2.3 Methodology 17
  - 2.4 Case Study 17
    - 2.4.1 Data 18
      - 2.4.2 Process Simulations and Economic Evaluation 19
        - 2.4.2.1 Changes in Fixed and Variable Costs 20
        - 2.4.2.2 Revenue 21
        - 2.4.2.3 Economic Calculations 21
      - 2.4.3 Safety Index Calculations 22
    - 2.5 Discussion 23

2.5.1	Process Simulations	23
2.5.1.1	Dehydration Process	23
2.5.1.2	NGL Recovery Process	23
2.5.1.3	Fractionation Train	26
2.5.1.4	Acid Gas Removal	26
2.5.2	Profitability Assessment	26
2.5.3	High Acid Gas Case Economics	30
2.5.4	Safety Index Results	30
2.5.5	Sensitivity Analysis	32
2.5.5.1	Heating Value Cases	33
2.5.5.2	NGL Price Cases	34
2.6	Conclusions	35
	Appendices	35
	2.A Appendix A: Key Parameters for the Dehydration Process	36
	2.B Appendix B: Key Parameters for the Turboexpander Process	36
	2.C Appendix C: Key Parameters for the Fractionation Train	37
	2.D Appendix D: Key Parameters for the Acid Gas Removal System	37
	References	39
<b>3</b>	<b>Sustainable Design and Model-Based Optimization of Hybrid RO–PRO Desalination Process</b>	<b>43</b>
	<i>Zhibin Lu, Chang He, Bingjian Zhang, Qinglin Chen, and Ming Pan</i>	
3.1	Introduction	43
3.2	Unit Model Description and Hybrid Process Design	47
3.2.1	The Process Description	47
3.2.2	Unit Model and Performance Metrics	49
3.2.2.1	RO Unit Model	49
3.2.2.2	PRO Unit Model	52
3.2.3	The RO–PRO Hybrid Processes	54
3.2.3.1	Open-Loop Configuration	54
3.2.3.2	Closed-Loop Configuration	55
3.3	Unified Model-Based Analysis and Optimization	56
3.3.1	Dimensionless Mathematical Modeling	56
3.3.2	Mathematical Model and Objectives	58
3.3.3	Optimization Results and Comparative Analysis	59
3.4	Conclusion	62
	Nomenclature	63
	References	65
<b>4</b>	<b>Techno-economic and Environmental Assessment of Ultrathin Polysulfone Membranes for Oxygen-Enriched Combustion</b>	<b>69</b>
	<i>Serene Sow Mun Lock, Kok Keong Lau, Azmi Mohd Shariff, Yin Fong Yeong, and Norwahyu Jusoh</i>	
4.1	Introduction	69
4.2	Numerical Methodology for Membrane Gas Separation Design	70
4.3	Methodology	73

4.3.1	Simulation and Elucidation of Mixed Gas Transport Properties of Ultrathin PSF Membranes (Molecular Scale)	73
4.3.2	Simulation of Mathematical Model Interfaced in Aspen HYSYS for Mass and Heat Balance (Mesoscale)	75
4.3.3	Design of Oxygen-Enriched Combustion Using Ultrathin PSF Membranes	75
4.4	Results and Discussion	77
4.4.1	Simulation and Elucidation of Mixed Gas Transport Properties of Ultrathin PSF Membranes (Molecular)	77
4.4.2	Simulation of Mathematical Model Interfaced in Aspen HYSYS for Mass and Heat Balance (Mesoscale)	79
4.4.3	Design of Oxygen-Enriched Combustion Using Ultrathin PSF Membranes	82
4.4.3.1	Membrane Area Requirement	82
4.4.3.2	Compressor Power Requirement	83
4.4.3.3	Turbine Power Requirement	85
4.4.3.4	Economic Parameter	88
4.5	Conclusion	90
	Acknowledgment	91
	References	91
<b>5</b>	<b>Process Intensification of Membrane-Based Systems for Water, Energy, and Environment Applications</b>	<b>97</b>
	<i>Nik A. H. M. Nordin, Zulfan A. Putra, Muhammad R. Bilad, Mohd D. H. Wirzal, Lila Balasubramaniam, Anis S. Ishak, and Sawin Kaur Ranjit Singh</i>	
5.1	Introduction	97
5.2	Membrane Electrocoagulation Flocculation for Dye Removal	99
5.3	Carbonation Bioreactor for Microalgae Cultivation	102
5.4	Forward Osmosis and Electrolysis for Energy Storage and Treatment of Emerging Pollutant	107
5.5	Conclusions and Future Perspective	111
	References	113
<b>6</b>	<b>Design of Internally Heat-Integrated Distillation Column (HIDiC)</b>	<b>117</b>
	<i>Vasu Harvindran and Dominic C. Y. Foo</i>	
6.1	Introduction	117
6.2	Example and Conceptual Design of Conventional Column	119
6.3	Basic Design of HIDiC	120
6.4	Complete Design of HIDiC	122
6.4.1	Top-Integrated Column	122
6.4.2	Bottom-Integrated Column	123
6.4.3	Geometrical Analysis for Heat Panels	124
6.5	Energy Savings and Economic Evaluation	126
6.6	Concluding Thoughts	128
	References	128

<b>7</b>	<b>Graphical Analysis and Integration of Heat Exchanger Networks with Heat Pumps</b> 131
	<i>Minbo Yang and Xiao Feng</i>
7.1	Introduction 131
7.2	Influences of Heat Pumps on HENs 132
7.2.1	Case 1 133
7.2.2	Case 2 134
7.2.3	Case 3 134
7.2.4	Case 4 135
7.2.5	Case 5 136
7.2.6	Case 6 136
7.2.7	Case 7 136
7.3	Integration of Heat Pump Assisted Distillation in the Overall Process 138
7.3.1	Increase of Pinch Temperature 138
7.3.2	Decrease of Pinch Temperature 140
7.3.3	No Change in Pinch Temperature 141
7.3.4	Heat Pump Placement 142
7.4	Case Study 145
7.5	Conclusion 148
	References 148
<b>8</b>	<b>Insightful Analysis and Integration of Reactor and Heat Exchanger Network</b> 151
	<i>Di Zhang, Guilian Liu, and Xiao Feng</i>
8.1	Introduction 151
8.2	Influence of Temperature Variation on HEN 152
8.2.1	Location of Cold and Hot Streams 152
8.2.2	Effect of Temperature Variation 153
8.3	Relation Among Reactor Parameters 156
8.3.1	Relation Among Temperatures, Selectivity, and Conversion of Reactor 157
8.3.1.1	CSTR 159
8.3.1.2	PFR 159
8.3.2	Reactor Characteristic Diagram 160
8.4	Coupling Optimization of HEN and Reactor 161
8.5	Case Study 163
8.6	Conclusions 165
	References 166
<b>9</b>	<b>Fouling Mitigation in Heat Exchanger Network Through Process Optimization</b> 167
	<i>Yufei Wang and Xiao Feng</i>
9.1	Introduction 167
9.2	Operation Parameter Optimization for Fouling Mitigation in HENs 169
9.2.1	Description on Velocity Optimization 169

9.2.2	Fouling Threshold Model	171
9.2.3	Heat Transfer Related Models	172
9.2.4	Pressure Drop Related Models	174
9.3	Optimization of Cleaning Schedule	175
9.4	Application of Backup Heat Exchangers	175
9.5	Optimization Constraints and Objective Function	176
9.5.1	Optimization Constraints	176
9.5.2	Objective Function	177
9.5.3	Optimization Algorithm	178
9.6	Case Studies	178
9.6.1	Case Study 1: Consideration of Velocity Optimization Alone	178
9.6.1.1	Optimization Results	180
9.6.2	Case Study 2: Simultaneous Consideration of Velocity and Cleaning Schedule Optimization	186
9.6.2.1	Constraints for Case Study	188
9.6.2.2	Results and Discussion	189
9.6.2.3	Considering Backup Heat Exchanger	194
9.7	Conclusion	194
	Acknowledgments	196
	References	198
<b>10</b>	<b>Decomposition and Implementation of Large-Scale Interplant Heat Integration</b>	<b>201</b>
	<i>Runrun Song, Xiao Feng, Mahmoud M. El-Halwagi, and Yufei Wang</i>	
10.1	Introduction	201
10.1.1	Reviews and Discussions for Stream Selection	202
10.1.2	Reviews and Discussions for Plant Selection	204
10.1.3	Reviews and Discussions for Plant Integration	204
10.2	Methodology	205
10.2.1	Strategy 1 – Overview	205
10.2.2	Identification of Heat Sources/Sinks for IPHI from Individual Plants	206
10.2.3	Decomposition of a Large-Scale IPHI Problem into Small-Scale Subsections	207
10.2.4	Strategy 2 for Indirect IPHI	209
10.3	Case Study	212
10.3.1	Example 1	212
10.3.2	Example 2	215
10.4	Conclusion	217
	References	218
<b>11</b>	<b>Multi-objective Optimisation of Integrated Heat, Mass and Regeneration Networks with Renewables Considering Economics and Environmental Impact</b>	<b>221</b>
	<i>So-Mang Kim, Adeniyi J. Isafade, and Michael Short</i>	
11.1	Introduction	221
11.2	Literature Review	222

11.2.1	Regeneration in Process Synthesis	222
11.2.2	The Analogy of MEN and REN	222
11.2.3	Combined Heat and Mass Exchange Networks (CHAMENs)	224
11.3	Environmental Impact in Process Synthesis	225
11.3.1	Life Cycle Assessment	225
11.4	The Synthesis Method and Model Formulation	226
11.4.1	Synthesis Approach	227
11.4.2	Assumptions	229
11.4.3	MINLP Model Formulation	230
11.4.3.1	HENS Model Equations	230
11.4.3.2	MEN and REN Model Equations	233
11.4.3.3	The Combined Economic Objective Function	236
11.4.3.4	Initializations and Convergence	239
11.5	Case Study	240
11.5.1	H <sub>2</sub> S Removal	240
11.5.1.1	Synthesis of MEN (The First Step)	242
11.5.1.2	Simultaneous Synthesis of MEN and REN (The Second Step)	243
11.5.1.3	Simultaneous Synthesis of MEN, REN, and HEN (The Third Step)	244
11.5.1.4	Absorption and Regeneration Temperature Optimization	247
11.5.1.5	The Synthesis of Combined Model Using MOO	252
11.6	Conclusions and Future Works	254
	References	256

## **12 Optimization of Integrated Water and Multi-regenerator Membrane Systems Involving Multi-contaminants: A Water-Energy Nexus Aspect**

*Musah Abass and Thokozani Majozi*

12.1	Introduction	261
12.2	Problem Statement	263
12.3	Model Formulation	263
12.3.1	Material Balances for Sources	264
12.3.2	Mass and Contaminants Balances for Regeneration Units	265
12.3.3	Mass and Contaminant Balances for Permeate and Reject Streams	265
12.3.4	Mass and Contaminant Balances for Sinks	266
12.3.5	Modeling of the Regeneration Units	266
12.3.5.1	Performance of Regeneration Units	266
12.3.6	Logical Constraints	267
12.3.7	The Objective Function	267
12.4	Illustrative Example	268
12.5	Conclusion	272
	Acknowledgments	272
	12.A Appendix: Detailed Models for the ED and RO Modules	273
	Nomenclature	280
	References	282

<b>13</b>	<b>Optimization Strategies for Integrating and Intensifying Housing Complexes</b>	<b>285</b>
	<i>Jesús M. Núñez-López, and José M. Ponce-Ortega</i>	
13.1	Introduction	285
13.2	Methods	288
13.2.1	Total Annual Cost for the Integrated System	289
13.2.2	Fresh Water Consumption	289
13.2.3	GHGE Emissions	290
13.2.4	Environmental Impact	290
13.2.5	Sustainability Return of Investment	293
13.2.6	Process Route Healthiness Index	293
13.2.7	Multistakeholder Approach	295
13.3	Case Study	295
13.4	Results	296
13.5	Conclusions	296
	References	299
<b>14</b>	<b>Sustainable Biomass Conversion Process Assessment</b>	<b>301</b>
	<i>Eric C. D. Tan</i>	
14.1	Introduction	301
14.2	Methodology and Assumptions	302
14.3	Results and Discussion	305
14.3.1	Environmental Indicators	305
14.3.2	Energy Indicators	310
14.3.3	Efficiency Indicators	312
14.3.4	Economic Indicators	313
14.4	Conclusions	314
	Acknowledgments	316
	References	317
	<b>Index</b>	<b>319</b>

