

Contents

Preface — V

List of Contributors — XIV

Editor Biography — XVI

Ben-Guang Rong

1	Introduction to basic concepts and elements in process synthesis and process intensification — 1
1.1	Introduction — 1
1.2	Basic elements in synthesis and intensification of distillation systems — 3
1.3	Basic facets of process synthesis — 4
1.3.1	Introduction to process synthesis — 4
1.3.2	Two approaches for finding alternatives in process synthesis: pure synthesis versus practical synthesis — 7
1.4	Basic facets of process intensification — 9
1.5	Evaluation indicators for PS and PI works — 11
1.6	Concepts of process synthesis work and process intensification work — 12
1.7	Conceptual design of process and equipment — 13
1.8	Concepts of the system and technical system — 14
1.8.1	System concept — 15
1.8.2	Technical system concept — 16
1.9	Software and hardware systems for a technical system — 18
1.9.1	Software elements — 18
1.9.2	Hardware elements — 19
1.9.3	Emergence of the technical system — 21
1.10	Triple parties in the working process of the methodology: the subject, object, and scientific method — 21
1.11	Synthesis and analysis as basic scientific methods — 23
1.11.1	Synthesis-dominated versus analysis-dominated methods — 23
1.11.2	Synthesis and analysis as basic methods in PS and PI works — 25
1.11.3	Process synthesis versus process analysis — 26
1.12	Systematic procedure as an element — 28
1.12.1	General procedures for process synthesis — 29
1.12.2	Specific procedures for PS and PI — 29
1.13	Concept of the technical system as a technology whole — 30
1.14	Example: the basic elements addressed in distillation intensification for the dividing-wall column subspace — 34
1.15	Conclusions — 39
1.16	Bibliography — 39

Ben-Guang Rong

2	Process synthesis and process intensification for multicomponent distillation systems – systematic methodology — 41
2.1	Introduction — 41
2.2	Problem definition — 44
2.2.1	Multicomponent mixtures — 44
2.2.2	Product specifications — 45
2.3	Dominant criteria for evaluation of a distillation system — 45
2.4	Basic concepts for multicomponent distillations — 45
2.4.1	Sharp and nonsharp splits — 45
2.4.2	Simple distillation column — 46
2.5	Basic software and hardware elements for a distillation system — 47
2.5.1	Software elements — 47
2.5.2	Hardware elements — 49
2.6	Distinct separation sequences — 50
2.7	Subspace of sharp sequence configurations — 52
2.8	Subspace of nonsharp sequence configurations — 54
2.9	Subspace of the original thermally coupled configurations — 62
2.10	Subspace of the thermodynamically equivalent structures — 68
2.11	Intensified distillation systems with fewer columns — 74
2.11.1	Subspace of the intensified simple column configurations — 75
2.11.2	Subspace of intensified distillation systems — 82
2.12	Subspace of dividing-wall columns — 90
2.12.1	DWCs from thermodynamically equivalent structures with side columns — 91
2.12.2	DWCs from prefractionation columns — 97
2.13	Summary and remarks — 103
2.13.1	Primary results — 103
2.13.2	Distinct subspaces for multicomponent distillation — 104
2.13.3	About the subspaces and their relationships — 104
2.13.4	About the method scopes of the subspaces for process synthesis and process intensification — 105
2.13.5	About the mechanisms and systematic procedures — 105
2.13.6	Common elements of the methods for distillation subspaces — 105
2.13.7	About further studies and applications — 106
2.14	Conclusions — 107
2.15	Nomenclature — 107
2.16	Bibliography — 108

Adriana Freites Aguilera, Pasi Tolvanen, Victor Sifontes Herrera, Jean-Noël Tourviele, Sébastien Leveneur, and Tapio Salmi

- 3 Reaction intensification by microwave and ultrasound techniques in chemical multiphase systems — 111**
 - 3.1 Microwave irradiation — 111
 - 3.1.1 Background — 111
 - 3.1.2 Heating mechanisms — 113
 - 3.1.3 Dielectric loss and permittivity — 114
 - 3.1.4 Selective heating — 115
 - 3.1.5 Case 1: conventional heating versus microwaves for epoxidation of vegetable oils — 117
 - 3.1.6 Case 2: effect of resonant microwave fields on temperature distribution in time and space — 119
 - 3.2 Process intensification by ultrasound: sonochemistry — 124
 - 3.2.1 What is ultrasound? — 124
 - 3.2.2 Ultrasonification techniques — 126
 - 3.2.3 Case 1: catalyst activation by ultrasonification — 127
 - 3.2.4 Ultrasonification of starch — 135
 - 3.3 Conclusions — 138
 - 3.4 Bibliography — 138

Anton A. Kiss

- 4 Process intensification by reactive distillation — 143**
 - 4.1 Introduction — 143
 - 4.2 Principles of reactive distillation — 144
 - 4.3 Modeling reactive distillation — 147
 - 4.3.1 Residue curve map — 149
 - 4.4 Design and control — 152
 - 4.5 Reactive distillation equipment — 161
 - 4.6 Applications of reactive distillation — 163
 - 4.7 Case study: biodiesel production by heat-integrated reactive distillation — 163
 - 4.8 Case study: fatty esters synthesis by dual reactive distillation — 169
 - 4.9 Case study: industrial reactive distillation process for methyl acetate production — 173
 - 4.10 Concluding remarks — 176
 - 4.11 Bibliography — 177

Massimiliano Errico

- 5 Process synthesis and intensification of hybrid separations — 182**
 - 5.1 Introduction — 182
 - 5.2 Pervaporation-assisted distillation — 185

5.2.1	Hybrid distillation/pervaporation processes for bioethanol purification —	189
5.2.2	Hybrid distillation/pervaporation processes for biobutanol purification —	192
5.2.3	Hybrid distillation/pervaporation processes: final remarks —	194
5.3	Liquid–liquid extraction-assisted distillation —	195
5.3.1	Hybrid liquid–liquid extraction/distillation processes for bioethanol purification —	197
5.3.2	Hybrid liquid–liquid extraction/distillation processes for biobutanol purification —	199
5.3.3	Hybrid liquid–liquid extraction/distillation processes: final remarks —	201
5.4	Synthesis, design, and optimization of alternative hybrid configurations for biobutanol separation —	202
5.5	Conclusions —	207
5.6	Bibliography —	208

Petri Uusi-Kyyny, Saeed Mardani, and Ville Alopaeus

6	Process intensification for microdistillation using the equipment miniaturization approach —	213
6.1	Introduction —	213
6.2	Development of small-scale distillation units —	217
6.2.1	Reflux ratio control —	219
6.2.2	Reboiler types —	220
6.3	Distillation column structures —	221
6.3.1	Brass column with heat pipe type of operation —	221
6.3.2	Stainless steel plate type of column —	222
6.3.3	Modular copper column —	223
6.3.4	Laser-welded square column —	224
6.3.5	3D-printed coiled compact distillation column —	225
6.3.6	3D-printed modular coiled distillation column —	226
6.3.7	Conclusion of distillation column structure review —	228
6.4	Metal foam as a packing material —	229
6.5	3D-printed packings —	231
6.6	Application of microscale distillation for small-scale piloting —	231
6.6.1	Distillation model —	233
6.6.2	Process model —	233
6.6.3	Apparatus and instrumentation —	234
6.6.4	Impurity accumulation test —	236
6.6.5	Conclusions from the small-scale pilot test runs —	236
6.7	Conclusions —	238
6.8	Bibliography —	239

Carlo Edgar Torres-Ortega and Ben-Guang Rong

7	Integrated biofuels process synthesis: integration between bioethanol and biodiesel processes — 241
7.1	Introduction — 241
7.1.1	Energy world consumption projections — 241
7.1.2	Worldwide transportation sector — 242
7.1.3	Biofuel potential — 243
7.1.4	Rural and industrial market and development — 244
7.1.5	Environmental situation — 245
7.1.6	Fuel properties of bioethanol and biodiesel — 246
7.2	Lignocellulosic bioethanol production process — 247
7.2.1	Biomass handling — 248
7.2.2	Pretreatment of lignocellulosic materials — 250
7.2.3	Hydrolysis of cellulose and hemicellulose, and fermentation strategies — 250
7.2.4	Separation and dehydration of bioethanol — 251
7.3	Fatty acid ethyl esters: biodiesel production process — 253
7.3.1	Extraction and conversion of oils — 255
7.3.2	Conversion of oil into alkyl esters — 255
7.3.3	Separation and purification of biodiesel — 257
7.3.4	New uses for glycerol — 258
7.4	Integration between bioethanol and biodiesel processes — 258
7.4.1	Mass integration — 260
7.4.2	Energy integration — 261
7.4.3	Integration between units → intensification — 262
7.5	Methodological framework for synthesis and intensification — 263
7.5.1	First stage: formulating and solving the superstructure synthesis problem through MINLP — 265
7.5.2	Second stage: intensification through recombination of column sections — 267
7.6	Case study: integrated lignocellulosic bioethanol and biodiesel process synthesis — 269
7.6.1	Problem description for superstructure optimization — 270
7.6.2	Superstructure setting and MINLP solution — 271
7.6.3	Synthesis-intensification: column section methodology — 276
7.6.4	Evaluation with the process simulator — 279
7.7	Discussions — 283
7.8	Conclusions — 284
7.9	Bibliography — 285

Chandrakant R. Malwade, Haiyan Qu, Ben-Guang Rong, and Lars P. Christensen

8	Process synthesis for natural products from plants based on PAT methodology — 290
8.1	Introduction — 290
8.1.1	Natural products from plants — 290
8.1.2	Need for recovery of natural products from plants — 294
8.1.3	Challenges in recovery of natural products from plants — 295
8.1.4	Process synthesis for separation of multicomponent mixtures — 297
8.2	Process synthesis for recovery of natural products from plants — 299
8.2.1	Process analytical technology — 300
8.2.2	PAT-based methodology for recovery of natural products from plants — 304
8.3	Recovery of artemisinin from <i>Artemisia annua</i> – a case study — 309
8.3.1	Generation of initial process flowsheet — 310
8.3.2	Evaluation of initial process flowsheet — 316
8.3.3	Measurement of solid–liquid equilibrium of artemisinin and impact of impurities — 317
8.3.4	Generation of improved process flowsheet — 319
8.4	Conclusions — 320
8.5	Bibliography — 322

Yufei Wang and Xiao Feng

9	Process synthesis for energy efficiency based on the pinch analysis approach — 325
9.1	The hierarchy of process synthesis — 325
9.2	Heat exchanger networks — 326
9.2.1	Pinch and energy targets — 326
9.2.2	Capital cost-related targets — 330
9.2.3	Synthesis of HENs — 331
9.2.4	HEN synthesis example — 333
9.2.5	Retrofit of HENs — 336
9.3	Utility selection — 340
9.3.1	Grand composite curve — 340
9.3.2	Utility selection — 342
9.3.3	Combined heat and power generation — 344
9.3.4	Integration of heat pumps — 346
9.4	Heat integration of reactors and distillation columns — 348
9.4.1	Appropriate placement of reactors — 348
9.4.2	Heat integration characteristics of a single distillation column — 350
9.4.3	Heat integration of a distillation system — 350
9.4.4	Appropriate placement of distillation column — 352

9.4.5	Use of the grand composite curve for heat integration of distillation column — 354
9.5	Heat integration across plants — 356
9.5.1	Total site profiles — 357
9.5.2	Direct and indirect heat integration — 358
9.5.3	Direct heat integration — 359
9.5.4	Indirect heat integration — 359
9.6	An industrial case study — 361
9.6.1	Procedure for energy integration for total site system retrofit — 361
9.6.2	Basic data for the case study — 362
9.6.3	HEN subsystem integration — 364
9.6.4	Separation subsystem integration and its coordination with HEN subsystem — 365
9.6.5	Coordination of HEN subsystem and utility subsystem — 366
9.6.6	Steam subsystem retrofit — 367
9.7	Concluding remarks — 368
9.8	Bibliography — 369

Juan Gabriel Segovia-Hernández, Fernando Israel Gómez-Castro, José Antonio Vázquez-Castillo, Gabriel Contreras-Zarazúa, and Claudia Gutiérrez Antonio

10 Process synthesis and intensification by integration between process design and control — 370

10.1	Introduction — 370
10.2	Process synthesis and integration of process design and control — 372
10.3	Closed-loop analysis — 376
10.3.1	Case study 1: reactive distillation to produce diphenyl carbonate — 377
10.3.2	Case study 2: thermally coupled distillation columns for the separation of a multicomponent mixture — 392
10.4	Conclusions — 400
10.5	Bibliography — 400

Index — 405