Contents

Preface ---- VII

About the author ---- IX

1	Introduction to sustainable processing —— 1
1.1	Sustainable development —— 2
1.2	Introduction to green chemistry —— 4
1.3	The 24 principles of green chemistry and green engineering —— 5
	Bibliography —— 11
2	Green process metrics —— 13
2.1	Atom economy —— 13
2.2	Reaction mass efficiency —— 15
2.3	Carbon efficiency —— 15
2.4	Effective mass yield —— 16
2.5	Environmental factor —— 16
2.6	Mass intensity —— 19
2.7	Process mass intensity —— 20
2.8	Mass productivity —— 20
2.9	Wastewater intensity —— 21
2.10	Solvent intensity —— 21
2.11	Carbon footprint, carbon emission factor, and carbon intensity —— 22
2.11.1	Methodology for carbon footprint industrial standards —— 23
2.11.2	Carbon footprint in the pharmaceutical industry —— 24
2.11.3	Carbon footprint in the petrochemical industry —— 25
2.12	Health and safety hazards —— 27
2.13	Defining a good chemical process —— 28
	Bibliography —— 30
3	The role of solvents in sustainable processes —— 32
3.1	Classification of solvents —— 33
3.2	Solvent usage and safety concerns —— 34
3.3	Green solvents —— 37
3.4	Solvent selection guides —— 42
	Bibliography —— 45
4	Sustainable process development from alpha to omega —— 48
4.1	PolarClean: a green polar aprotic solvent —— 48
4.2	The patented production of PolarClean —— 49
4.3	Toward the design of greener synthetic routes —— 51



4.4	Quality assessment —— 54
4.5	Green metrics analysis — 56
4.5.1	Complexity and Ideality —— 56
4.5.2	Carbon intensity —— 57
4.5.3	Atom economy —— 60
4.5.4	Yield —— 63
4.5.5	E-factors —— 65
4.5.6	Health and safety risks —— 66
4.5.7	Solvent intensity —— 68
4.6	Room for improvement: Further optimization potential —— 69
	Bibliography —— 70
5	Process intensification: methods and equipment —— 72
5.1	Evolution of chemical processes —— 77
5.2	Process-intensifying equipment —— 78
5.2.1	Microreactors —— 78
5.2.2	Rotating devices —— 80
5.3	Process-intensifying methods —— 83
5.3.1	Membrane reactors —— 84
5.3.2	Hybrid separations —— 86
5.3.3	Use of alternative energy: ultrasound and microwave —— 87
5.3.4	Other methods —— 92
	Bibliography —— 93
6	Continuous microflow processes —— 98
6.1	Introduction —— 98
6.2	The advantages and disadvantages of continuous microfluidic
	systems —— 100
6.3	The green attributes of continuous flow processes —— 102
6.3.1	Principle 1: Prevention —— 103
6.3.2	Principle 2: Atom economy —— 106
6.3.3	Principle 6: Design for energy efficiency —— 109
6.3.4	Principle 9: Catalysis —— 109
6.3.5	Principle 11: Real-time analysis for pollution prevention —— 111
6.3.6	Principle 12: Safer chemistry for accident prevention —— 112
6.4	Microflow reactor systems —— 114
6.5	Lab-of-the-future and automated robotic platforms —— 116
	Bibliography —— 117
7	Continuous separation processes —— 121
7.1	Downstream processing in organic synthesis —— 121
7.2	Batch versus continuous separations —— 121

7.3	Continuous processing with supercritical fluids —— 123
7.4	Continuous membrane separations —— 125
7.5	Continuous crystallization processes —— 132
7.6	Centrifugal partition chromatography —— 135
7.7	Pressure and temperature swing adsorption —— 137
7.8	Artificial intelligence in chemical and separation technologies —— 141
	Bibliography —— 143
8	Solvent recovery and recycling —— 147
8.1	Distillation processes —— 148
8.2	Adsorption processes —— 152
8.3	Membrane-based solvent recovery processes and their comparison
	with distillation and adsorption —— 154
8.4	Tools for solvent recovery process design —— 161
	Bibliography —— 162
9	Process analytical technology —— 165
9.1	Introduction —— 165
9.2	PAT for green chemistry and engineering —— 167
9.3	Development of PAT systems —— 170
9.4	Industry outlook —— 172
9.5	PAT methods —— 173
9.5.1	Infrared spectroscopy —— 173
9.5.2	Raman spectroscopy —— 175
9.5.3	Nuclear magnetic resonance spectroscopy —— 175
9.5.4	Ultraviolet-visible spectroscopy —— 176
9.6	Case studies —— 177
9.6.1	Control of ammonia content and reaction monitoring with FTIR —— 177
9.6.2	FTIR spectroscopy-enabled control strategy for brivanib alaninate
	manufacturing —— 180
9.6.3	Implementation of Raman spectroscopy in reaction monitoring —— 182
9.6.4	Process control of continuous synthesis and solid drug formulation by
	IR and Raman spectroscopy —— 183
	Bibliography —— 185
10	Sustainable nuclear fuels —— 188
10.1	Benefits of nuclear energy —— 192
10.2	Disadvantages of nuclear energy —— 193
10.3	Uranium as a nuclear fuel —— 195
10.3.1	Availability of uranium —— 195

10.3.2	Current methods for uranium sourcing —— 195
10.3.3	Sustainable extraction of uranium from seawater —— 197
10.4	Waste management —— 201
	Bibliography —— 204
11	Toward sustainable biofuel production processes —— 207
11.1	Production of alcohols as fuels —— 208
11.1.1	Biochemical conversion of lignocellulosic biomass —— 210
11.1.2	Grinding —— 210
11.1.3	Pretreatment —— 211
11.1.4	Hydrolysis/saccharification —— 212
11.1.5	Fermentation —— 213
11.1.6	Distillation/dehydration —— 214
11.1.7	Case study of a membrane integrated bioreactor system for the
	continuous production of bioethanol —— 215
11.2	Biodiesel and its conventional production —— 217
11.2.1	Alternative routes for biodiesel production —— 220
	Bibliography —— 225
12	Green polymers and green building blocks —— 229
12.1	Introduction —— 229
12.2	Polymers and the environment —— 231
12.3	Plastic waste management: methods and limitations —— 235
12.4	Bioplastics —— 236
12.5	Green polymers —— 238
12.6	Green monomers and building blocks —— 241
12.7	Extraction methods —— 248
12.7.1	Mechano-catalytic depolymerization —— 248
12.7.2	Integrated conversion —— 249
12.7.3	Ultrasound-assisted radical depolymerization —— 251
12.7.4	Fermentation —— 252
12.7.5	Segmented continuous flow fractionation —— 253
12.8	New design technology concepts for advanced polymer materials —— 254
12.8.1	Reactor design configuration —— 255
12.8.2	Online monitoring —— 255
12.8.3	Automation —— 256
12.8.4	Membranes —— 256
12.8.5	Membranes from chitosan and PLA —— 258
12.8.6	Production of bio-based polyethylene (bio-PE) —— 260
12.8.7	Bio-based 1,4-butanediol —— 262
12.8.8	BioFoam —— 263
12.8.9	Desmodur eco N —— 263

12.8.10	Rilsan HT and Rilsan Invent —— 264
12.8.11	Polycarbonates —— 264
	Bibliography —— 265
13	Solar powered engineering —— 269
13.1	Water harvesting from air —— 269
13.2	Solar-driven membrane processes —— 272
13.3	Concentrated solar power —— 275
13.4	Photochemistry and photocatalysis —— 279
13.4.1	Heterogeneous photocatalysis —— 280
13.4.2	Solar-driven advanced oxidation processes —— 283
13.4.3	Hybrid advanced oxidation processes —— 284
13.4.4	Homogeneous photocatalysis —— 286
13.4.5	Luminescent solar concentrator reactors —— 287
13.4.6	Cloud-inspired photochemical reactor —— 288
13.4.7	Chiral separation using light —— 290
	Bibliography —— 291
14	Data-driven optimization of chemical processes —— 294
14.1	Self-optimizing systems —— 295
14.1.1	Autonomous experimentation platforms —— 296
14.2	Fault detection and diagnosis systems in industrial processes —— 301
14.2.1	Shallow machine learning algorithms —— 303
14.2.2	Deep learning —— 305
14.2.3	Transfer learning —— 307
14.2.4	Unsupervised machine learning algorithms —— 309
14.3	Refinery production scheduling —— 310
14.3.1	Optimizing production scheduling: industry 3.0 vs. industry 4.0 in oil refinery operations —— 311
14.3.2	Challenges —— 315
14.3.3	Real case: Abqaiq Plants, a digital transformation success story —— 317
14.3.4	Enhancing heating control to increase refinery throughput —— 319
14.3.5	Model predictive control in scheduling a refinery —— 320
	Bibliography —— 323
15	Worked examples —— 327
15.1	Example 1 – Green metrics analysis for hazardous chemistry scale-up
	and decision-making —— 327
15.1.1	Part A problem statements —— 327
15.1.2	Part B problem statements —— 327
15.1.3	Part A solutions —— 328
15.1.4	Part B solutions —— 329

15.2	Example 2 – Green metric analysis of catalytic synthesis and
	purification of a pharmaceutical building block —— 332
15.2.1	Part A problem statements —— 332
15.2.2	Part B problem statements —— 332
15.2.3	Part A solutions —— 333
15.2.4	Part B solutions —— 334
15.3	Example 3 – Comparison of batch and microflow processes in
	diazomethane-based chemistry —— 336
15.3.1	Part A problem statements —— 336
15.3.2	Part B problem statements —— 337
15.3.3	Part A solutions —— 338
15.3.4	Part B solutions —— 342
15.4	Example 4 – Bioethanol production: conventional batch fermentation
	versus continuous membrane bioreactor 344
15.4.1	Part A problem statements —— 344
15.4.2	Part A solutions —— 345
15.4.3	Part B problem statements —— 348
15.4.4	Part B solutions —— 349
15.5	Example 5 – Application of process analytical technologies in
	continuous catalytic hydrogenation —— 354
15.5.1	Problem statements —— 354
15.5.2	Solutions —— 355
15.6	Example 6 – Green metrics analysis for hazardous chemistry and
	purification optimization —— 356
15.6.1	Part A problem statements —— 357
15.6.2	Part A solutions —— 357
15.6.3	Part B problem statements —— 358
15.6.4	Part B solutions —— 359
15.7	Example 7 – Green metrics analysis and reaction optimization —— 360
15.7.1	Part A problem statements —— 361
15.7.2	Part A solutions —— 361
15.7.3	Part B problem statements —— 362
15.7.4	Part B solutions —— 362
15.7.5	Part C problem statements —— 364
15.7.6	Part C solutions —— 364
15.7.7	Part D problem statements —— 365
15.7.8	Part D solutions —— 365
	Bibliography —— 366