

Contents

Preface — VII

About the author — IX

1	Introduction to sustainable processing — 1
1.1	Sustainable development — 1
1.2	Introduction to green chemistry — 4
1.3	The 24 principles of green chemistry and green engineering — 5
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 — 20
2.10	Solvent intensity — 21
2.11	Carbon footprint, carbon emission factor, and carbon intensity — 21
2.11.1	Methodology for carbon footprint industrial standards — 22
2.11.2	Carbon footprint in the pharmaceutical industry — 24
2.11.3	Carbon footprint in the petrochemical industry — 24
2.12	Health and safety hazards — 26
2.13	Defining a good chemical process — 28
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
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 —	62
4.5.5	E-factors —	63
4.5.6	Health and safety risks —	65
4.5.7	Solvent intensity —	67
4.6	Room for improvement: further optimization potential —	68
5	Process intensification: methods and equipment —	71
5.1	Evolution of chemical processes —	74
5.2	Process-intensifying equipment —	76
5.2.1	Microreactors —	77
5.2.2	Rotating devices —	80
5.3	Process-intensifying methods —	82
5.3.1	Membrane reactors —	83
5.3.2	Hybrid separations —	85
5.3.3	Use of alternative energy: ultrasound and microwave —	86
6	Continuous microflow processes —	95
6.1	Introduction —	95
6.2	The advantages and disadvantages of continuous microfluidic systems —	96
6.3	The green attributes of continuous flow processes —	98
6.3.1	Principle 1: prevention —	99
6.3.2	Principle 2: atom economy —	103
6.3.3	Principle 6: design for energy efficiency —	106
6.3.4	Principle 9: catalysis —	106
6.3.5	Principle 11: real-time analysis for pollution prevention —	108
6.3.6	Principle 12: safer chemistry for accident prevention —	108
6.4	Microflow reactor systems —	110
7	Continuous separation processes —	117
7.1	Downstream processing in organic synthesis —	117
7.2	Batch versus continuous separations —	117
7.3	Continuous processing with supercritical fluids —	119
7.4	Continuous membrane separations —	120
7.5	Continuous crystallization processes —	128
7.6	Centrifugal partition chromatography —	131
7.7	Pressure and temperature swing adsorption —	132
8	Solvent recovery and recycling —	141
8.1	Distillation processes —	142

8.2	Adsorption processes —	146
8.3	Membrane-based solvent recovery processes and their comparison with distillation and adsorption —	148
9	Process analytical technology —	158
9.1	Introduction —	158
9.2	PAT for green chemistry and engineering —	160
9.3	Development of PAT systems —	161
9.4	Industry outlook —	164
9.5	PAT methods —	165
9.5.1	Infrared spectroscopy —	165
9.5.2	Raman spectroscopy —	167
9.5.3	Nuclear magnetic resonance spectroscopy —	168
9.5.4	Ultraviolet-visible spectroscopy —	168
9.6	Case studies —	169
9.6.1	Control of ammonia content and reaction monitoring with FTIR —	170
9.6.2	FTIR spectroscopy-enabled control strategy for brivanib alaninate manufacturing —	172
9.6.3	Implementation of Raman spectroscopy in reaction monitoring —	174
9.6.4	Process control of continuous synthesis and solid drug formulation by IR and Raman spectroscopy —	175
10	Sustainable nuclear fuels —	181
10.1	Benefits of nuclear energy —	184
10.2	Disadvantages of nuclear energy —	186
10.3	Uranium as a nuclear fuel —	187
10.3.1	Availability of uranium —	188
10.3.2	Current methods for uranium sourcing —	188
10.3.3	Sustainable extraction of uranium from seawater —	189
10.4	Waste management —	194
11	Toward sustainable biofuel production processes —	200
11.1	Production of alcohols as fuels —	201
11.1.1	Biochemical conversion of lignocellulosic biomass —	203
11.1.2	Grinding —	203
11.1.3	Pretreatment —	204
11.1.4	Hydrolysis/saccharification —	205
11.1.5	Fermentation —	206
11.1.6	Distillation/dehydration —	207
11.1.7	Case study of a membrane integrated bioreactor system for the continuous production of bioethanol —	208
11.2	Biodiesel and its conventional production —	210

11.2.1	Alternative routes for biodiesel production —	213
12	Green polymers and green building blocks —	222
12.1	Introduction —	222
12.2	Polymers and the environment —	224
12.3	Plastic waste management: methods and limitations —	227
12.4	Bioplastics —	229
12.5	Green polymers —	231
12.6	Green monomers and building blocks —	234
12.7	Extraction methods —	241
12.7.1	Mechano-catalytic depolymerization —	241
12.7.2	Integrated conversion —	243
12.7.3	Ultrasound-assisted radical depolymerization —	243
12.7.4	Fermentation —	244
12.7.5	Segmented continuous flow fractionation —	246
12.8	New design technology concepts for advanced polymer materials —	247
12.8.1	Reactor design configuration —	248
12.8.2	Online monitoring —	248
12.8.3	Automation —	249
12.8.4	Membranes —	249
12.8.5	Membranes from chitosan and PLA —	251
12.8.6	Production of bio-based polyethylene (bio-PE) —	253
12.8.7	Bio-based 1,4-butanediol —	255
12.8.8	BioFoam —	256
12.8.9	Desmodur eco N —	256
12.8.10	Rilsan HT and Rilsan Invent —	257
12.8.11	Polycarbonates —	257
13	Solar powered engineering —	263
13.1	Water harvesting from air —	263
13.2	Solar-driven membrane processes —	265
13.3	Concentrated solar power —	269
13.4	Photochemistry and photocatalysis —	273
13.4.1	Heterogeneous photocatalysis —	274
13.4.2	Solar-driven advanced oxidation processes —	276
13.4.3	Hybrid advanced oxidation processes —	278
13.4.4	Homogeneous photocatalysis —	279
13.4.5	Luminescent solar concentrator reactors —	280
13.4.6	Cloud-inspired photochemical reactor —	282
13.4.7	Chiral separation using light —	284

14	Worked examples — 288
14.1	Example 1 – Green metrics analysis for hazardous chemistry scale-up and decision-making — 288
14.1.1	Part A problem statements — 288
14.1.2	Part B problem statements — 288
14.1.3	Part A solutions — 289
14.1.4	Part B solutions — 290
14.2	Example 2 – Green metric analysis of catalytic synthesis and purification of a pharmaceutical building block — 292
14.2.1	Part A problem statements — 293
14.2.2	Part B problem statements — 293
14.2.3	Part A solutions — 293
14.2.4	Part B solutions — 294
14.3	Example 3 – Comparison of batch and microflow processes in diazomethane-based chemistry — 296
14.3.1	Part A problem statements — 297
14.3.2	Part B problem statements — 298
14.3.3	Part A solutions — 299
14.3.4	Part B solutions — 302
14.4	Example 4 – Bioethanol production: conventional batch fermentation versus continuous membrane bioreactor — 304
14.4.1	Part A problem statements — 304
14.4.2	Part A solutions — 305
14.4.3	Part B problem statements — 308
14.4.4	Part B solutions — 309
14.5	Example 5 – Application of process analytical technologies in continuous catalytic hydrogenation — 314
14.5.1	Problem statements — 314
14.5.2	Solutions — 315

Index — 317
