Index

additives, 284. See growth inhibitors
agglomeration, 130
cementing of aggregates, 142
collision of particles, 133
definitions, 130
disruption of aggregates, 141
mechanism
inertial collision rate, 136
orthokinetic collision rate, 134
perikinetic collision rate, 134
modeling, 156
agglomeration kernel, 156
rate of, 156
the agglomeration kernel, 142
particle interaction, 140
transport of particles, 133
aggregation. See agglomeration
anti-solvent crystallization, 255. See also
crystallization method
batch crystallization, 178
cooling trajectory, 186
critical seed loading, 182
modeling, 185
optimal trajectory, 187
process design, 59
seed load, 181
seed quality, 184
seed size, 181
seeding procedure, 181
timing of the seed point, 184
coagulation. See agglomeration
coalessence. See agglomeration
cocrystals. See polymorph cocrystals
crystal growth. See growth rate
crystal habit. See crystal shape
crystal morphology. See also crystal shape
crystal faces, 35
prediction, 37
relation to crystal shape, 35

crystal shape, xxv, 35, 52
definition shape factors, 27
effect operating conditions, 40
effects additives, 40, 284
effects impurities, 40, 284
effects metal ions, 296
effects solvent, 284
FBRM, 197
light diffraction, 196
Miller indices, 36
polymorphism, 306
prediction, 37, 291
tomahawk, 292
crystal size
definition, 27
length, 27
projected area diameter, 27
shape factor, 27
sieve diameter, 27
surface diameter, 27
volume diameter, 27
crystal size distribution (CSD), xxiii, xxv, xxvi, 26, 31, 93
average crystal size, 27
coefficient of variation, 33
cumulative mass function M(L), 30
cumulative number function N(L), 30
dilution, 192
evolution of, 151
histogram, 31
mass-based mean size, 32
mass density m(L), 29
measuring techniques, 192, 193
backward light scattering, 197
dynamic light scattering, 194
FBRM, 197
forward light scattering, 195
imaging, 197
sieving, 193
the Coulter counter, 194
ultrasonic attenuation, 196
median crystal size L50, 32, 92
mode Ld, 32
modeling. See population balance moments of the distribution, 27, 31
number-based mean size, 32
number density \( n(L) \), 29
quartile ratio, 33
representation of, 28
sampling, 192
width of the distribution, 27, 33
crystallization method
anti-solvent, xxvii, 9, 54, 255
cooling, 7, 53
evaporative, 8, 11, 53
melt, xxv, xxvii, 4, 6, 53, 261
precipitation, 9, 54
product quality, 13
selection, 11, 53
crystallizer, xxiv
modeling, 168
scale-up, 168, 171
selection criteria, 210
type
cascade of crystallizers, 231
cooling disk, 229
direct cooling crystallizer, 228
draft tube baffle crystallizer, 217
draft tube crystallizer, 215
fluidized bed, 225
forced circulation, 220
growth crystallizer, 227
Oslo, 225
solar pond, 212
spray crystallizer, 228
surface cooling, 229
thermo-syphon, 213
crystallizer modeling
DTB crystallizer, 168, 170
density measuring. See supersaturation measuring techniques
depreciation period, 64
design
crystallization method
selection, 53
crystallization process, xxv, 51
crystallizer, xxv, 51
circulation flow rate, 62
dimensions, 60
eutriation leg, 63, 222
fines removal, 62
Karena nozzle, 222
maximal heat flux, 62
maximum vapor velocity, 61
product classification, 63
selection, 60
suspension criterion, 63
volume, 60
depreciation period, 64
economic evaluation, 64
flow sheet
calculations, 57
development, 55
equations, 57
solution method, 59
number of crystallization steps, 55
operation costs, 64
operation mode, 55
procedure, 51
process specifications, 52
product performance, 52
production rate \( P \), 59
profit, 65
residence time, 56
solubility, 53
solvent selection, 53
dissolution, 123
dynamic light scattering. See crystal size distribution (CSD) measuring techniques
energy consumption
evaporative crystallization, 54
eutectic freeze crystallization, 274
evaporative crystallization. See crystallization
FBRM. See crystal size distribution (CSD) measuring techniques
fines removal. See design crystallizer
flocculation. See agglomeration
forward light scattering. See crystal size distribution (CSD): measuring techniques
FTIR spectroscopy. See supersaturation measuring techniques
growth inhibitors. See growth inhibitors
anti-freeze proteins, 296
mechanisms
large organic molecules, 285
small organic molecules, 285
tailor-made additives, 287
metal ions, 296
molecular modeling, 288
applications, 290
polyelectrolytes, 293
small anions, 298
growth rate
basic concepts, 104
mechanism, 120
mechanism, 119
linear growth rate, 104
measurement, 124
mechanism, 105
birth and spread (B&S), 110
macro building blocks, 123
rough growth, 112
growth rate (cont.)
smooth growth, 107
spiral growth, 108
surface integration, 107
thermal roughening, 113
volume diffusion control, 115
size-dependent growth, 121
surfaces, 106
hydrates. See polymorphy hydrates
imaging. See crystal size distribution (CSD): measuring techniques
impurities. See mother liquor inclusions
Kolmogorov length scale, 137
liquid fraction $\varepsilon$, 59
maximal heat flux, 62
measuring techniques
crystal size distribution. See crystal size distribution (CSD)
supersaturation, 14, 234. See supersaturation
melt crystallization, 261. See crystallization
advantages, 262
definitions, 262
from suspension, 269
cooling profile, 270
crystallizers, 269
wash columns, 269, 272
impurity distribution, 263
phase diagrams, 263
solid layer, 265
cooling profile, 266
sweating, 268
technique
layer growth, 261
suspension growth, 261
metastable zone, 200, 275, 309
definition, 79
measurement, 79, 204
seed point, 179
Miller indices. See crystal shape
moment model. See population balance equation
morphology. See crystal morphology
mother liquor inclusions, xxv
nucleation, xxv, 71
induction time, 78
primary, 71
heterogeneous, 77
homogeneous, 71, 77
nucleation rate, 75
nucleus, 72
two-step mechanism, 83
rate measurement, 80
secondary, 89
mechanism: attrition breeding, 90; catalytic
breeding, 90; contact nucleation, 90;
dendritic breeding, 90; fluid shear breeding,
90; initial breeding, 90; needle breeding, 90
models: attrition model, 96; collision model,
92; power law, 91
operation costs, 64
organic growth inhibitors. See growth inhibitors
particle size distribution (PSD). See crystal size
distribution (CSD)
polymorphism, 303
polymorph
cocrystals, 315
formation kinetics, 309
hydrates, 314
seeding, 311
solvates, 314
systems
enantiotropic, 307
monotropic, 307
templates, 311
population balance equation, 151
formulation of, 153
solutions
MSMPR, 160
numerical solutions, 167
stationary operation, 159
the moment model, 164
stationary operation, 159
the boundary condition, 154
the initial conditions, 154
population balance equation, v, xxvi, 153
connection with material balance, 158
for agglomeration, 156
for breakage, 156
power input, 156
mean, 137
of stirrer, 63, 93
specific, 63, 64, 91, 93
precipitation, 234. See also crystallization: method
dominant phenomena, 236
mixing
configurations, 251
mechanisms, 237: macro-mixing, 238;
meso-mixing, 238; micro-mixing, 239
time and length scales, 240
modeling
compartment model, 243, 245
Eulerian method, 246
Lagrangian approach, 246
scale-up, 242
pressure melt crystallization, 274
product quality
modeling, 152
production rate, 52, 161, 184, 211, 213, 215, 217, 220, 226, 274
production rate P, 6, 58, 59, 65
profit, 65
Raman spectroscopic, 204
refractive index. See supersaturation: measuring
techniques
relative supersaturation. See supersaturation
shape. See crystal shape
shape factor, 28, 31, 105, 165
surface κs, 27
volumetric κv, 27
sieve analysis. See crystal size distribution (CSD):
measuring techniques
size. See crystal size
solubility, xxv
lines, 3
of polymorphs, xxviii
retrograde solubility, 9
salting out, 11
slope of solubility line, 6
sparingly soluble substances, 9
solubility
silver nitrate, 4
solubility decrease
anti solvent crystallization, 9
solvates. See polymorphism solvates
supersaturation, 14, 234
crystallization, 9
chemical potential difference, 15
crystal concentration M_T, 59
crystal volume, 165
density, 202
driving force, 1
local supersaturation, 168, 234
measuring techniques, 200
ATR-FTIR spectroscopy, 201
driving force, 1
mixing reagents, 237, 240
ratio S, 15
relative supersaturation σ, 16
speciation, 19
thermodynamic expression, 14
thermodynamic model, 1
selection, 21
thermodynamic models, 19
tailor made additives. See growth inhibitors
mechanisms
total crystal concentration M_T, 59
total crystal volume, 165
ultrasonic attenuation. See crystal size distribution
(CSD) measuring techniques
volumetric liquid fraction. See liquid fraction ε
Zel’dovich factor, 76, 111