

INDEX

A

- Adaptive Resonance Theory (ART)
 - clustering in process data interpretation, 63–64, 73–77, 92–93
 - input analysis of process data, 30–31
- Advection problem, solution, 109
- Affine deformation, drop breakup, 132–134
- Agglomerate, *see also* Aggregation; Fragmentation
 - definition, 159–160
 - flow type effect on separation following rupture, 165–167
 - particle interactions, 161–163
 - size distributions, 160, 181, 183–184
 - strength prediction, 164–165
- Aggregation, *see also* Agglomerate
 - bonding levels, 160–161
 - coalescence relationship, 106
 - diffusion-limited aggregation, 180–181
 - flow-induced aggregation
 - area-conserving cluster aggregation in two-dimensional chaotic flows, 189–190
 - cluster–cluster aggregation, 186
 - constant capture radius, aggregation in chaotic flows, 187, 189
 - features, 180–181, 186
 - fractal structure aggregation in chaotic flows, 191–192, 194
 - particle–cluster aggregation, 186
 - hierarchical cluster–cluster aggregation, 181
 - linear trajectory aggregation, 180–181
 - mass of clusters, 161
 - mechanisms, 180
 - polydispersity computations, 194
 - reaction-limited aggregation, 180–181
 - short-term behavior in well-mixed systems, 184–185
 - sizes, 160
- ART, *see* Adaptive Resonance Theory

B

- Back propagation network (BPN)
 - correspondence with linear discriminant pattern recognition, 53–55
 - input–output analysis of process data, 38–39
- Basis function
 - adaptive-shape basis functions, 13
 - fixed-shape basis functions, 12–13
- BPN, *see* Back propagation network
- Breakup
 - affine deformation, 132–134
 - capillary number, 130, 132
 - critical capillary number, 132, 134
 - drop size
 - daughter droplets, 143, 145
 - distribution from chaotic flows, 145, 147
 - viscosity ratio effect on distribution, 147, 149
 - flow reorientation importance, 134, 136
 - fragmentation relationship, 106–107
 - mechanisms
 - capillary instability, 141–143, 145, 149, 151, 195
 - combined mechanisms, 142
 - end-pinching, 139, 149
 - necking, 139, 143, 145, 149
 - tipstreaming, 139
 - modeling with coalescence, 155–159
 - satellite formation in capillary breakup, 143
 - small-scale mixing, 130–132
 - stretching of low-viscosity-ratio elongated drops, 137–138
 - thread breakup time during flow, 142–143
 - velocity field equations for common flow types, 131

C

- Capillary instability, *see* Breakup
- Capillary number
 - breakup problem, 130
 - critical capillary number, 132, 134
 - definition, 106, 128
- CART, *see* Classification and regression tree
- Catalytic converter, *see* Sulfur dioxide oxidation
- Cavity flow, characteristics, 110, 112–113
- Classification and regression tree (CART),
 - input–output analysis of process data, 41–42
- Clustering, process data interpretation
 - Adaptive Resonance Theory, 63–64, 73–77, 92–93
 - ellipsoidal basis function networks, 62–63
 - fixed cluster approaches, 61–63
 - generalization and memorization, 60
 - k-nearest neighbor rule, 59
 - kernel identification, 46
 - 1-nearest neighbor rule, 59
 - performance, 61
 - fixed cluster approaches, 61–63
 - proximity indices, 59
 - qualitative trend analysis, 63
 - radial basis function networks, 61–62
 - two-class problem example, 58–59
 - variable cluster approaches, 63–64
- Coalescence
 - aggregation relationship, 106
 - collisions
 - flow type effects on shear-induced collisions, 151–153, 155
 - frequency, 151, 155
 - film drainage, 153, 155
 - modeling with breakup, 155–159

D

- Data analysis
 - abnormal situation detection in
 - continuous polymer process, 82–86
 - batch operation variability, 86–90
 - challenges with process data
 - discriminant uncertainty, 8

- dynamic changes to process conditions, 8
 - lack of abnormal situation exemplars, 8
 - measurement uncertainty, 8
 - scale and scope of process, 7–8
- feature mapping
 - pattern exemplars, 4
 - training set, 4
- input mapping, *see* Input analysis, process data
- input–output mapping, *see* Input–output analysis, process data
- numeric–numeric transformation, 3
- pattern recognition, overview, 2–3
- Q-statistics, 90
- selection of techniques, 9
- Data interpretation
 - backpropagation network,
 - correspondence with linear discriminant pattern recognition, 53–55
 - challenges with process data
 - discriminant uncertainty, 8
 - dynamic changes to process conditions, 8
 - lack of abnormal situation exemplars, 8
 - measurement uncertainty, 8
 - scale and scope of process, 7–8
 - diagnosis of batch polymer reactor
 - operating problems, 90–96
 - hierarchical modularization, 79–82
 - hyperplane orientations, 49–50
 - knowledge-based system approaches
 - applications, 66–67
 - decomposition of complex problems, 72, 93–94
 - digraph, 70
 - fault tree, 69–70
 - feed injection system example, 65–66
 - model-based methods, 68–69
 - overview, 44, 64–65
 - semantic networks, 67
 - tables, 65, 67, 70–71
- labels
 - context dependence, 6–7
 - types, 5–6
- limit checking, 48–49
- local interpretation methods
 - clustering

- Adaptive Resonance Theory, 63–64, 73–77, 92–93
 - ellipsoidal basis function networks, 62–63
 - fixed cluster approaches, 61–63
 - generalization and memorization, 60
 - k-nearest neighbor rule, 59
 - kernel identification, 46
 - 1-nearest neighbor rule, 59
 - performance, 61
 - proximity indices, 59
 - qualitative trend analysis, 63
 - radial basis function networks, 61–62
 - two-class problem example, 58–59
 - variable cluster approaches, 63–64
 - probability density function approaches, 56–58
 - statistical measures for interpretation, 55–56
 - nonlocal interpretation methods
 - multivariate linear discriminant methods, 49–55
 - univariate methods, 47–49
 - numeric–symbolic mapping, 6, 43–55, 72–78
 - selection of techniques, 9
 - symbolic–symbolic mapping, 6, 64–72
 - Dispersion, *see* Powder dispersion in liquids
 - Duct flow
 - characteristics, 113–114
 - conversion into efficient mixing flows, 114, 116
 - velocity field, 113
- E**
- EBFN, *see* Ellipsoidal basis function network
 - Ellipsoidal basis function network (EBFN)
 - clustering in process data interpretation, 62–63
 - input analysis of process data, 30
 - End-pinching, *see* Breakup
 - Erosion, *see* Fragmentation
- F**
- FCCU, *see* Fluidized catalyst cracking unit
 - Flocculation, *see* Aggregation
- F**
- Fluidized catalyst cracking unit (FCCU),
 - input process data interpretation
 - Adaptive Resonance Theory degradation with complexity, 73–77
 - fast ramp training scenario, 73–74
 - hierarchical decomposition of
 - malfunction groupings, 74–77
 - malfunction types, 73
 - slow ramp malfunction scenario, 73–74
 - Fragmentation, *see also* Agglomerate
 - breakup relationship, 106–107
 - definition, 160
 - deformation of agglomerates, 163
 - dispersion kinetics in two-zone model, 170–171, 173
 - distribution of fragments, 163
 - erosion
 - definition, 160, 179–180
 - kinetics, 169–170, 176–178
 - simultaneous rupture, 173, 178–179
 - fragmentation number, 106, 164
 - particle size distribution analysis, 173–176
 - rupture
 - critical fragmentation number, 167–169
 - definition, 160, 180
 - simultaneous erosion, 173, 178–179
 - scaling solutions of fragmentation equation, 107
 - shattering, 160
- G**
- Gel permeation chromatography (GPC),
 - diagnosis of batch polymer reactor operating problems, 91–95
 - GPC, *see* Gel permeation chromatography
- H**
- Hierarchical classification, process data interpretation, 80
 - Horseshoe map, chaotic mixing, 110
- I**
- Immiscible fluid mixing
 - breakup, *see* Breakup

Immiscible fluid mixing (*Continued*)

- coalescence, *see* Coalescence
 - dispersed fluid phases, role in flow structure, 129–130
 - initial stages, 128–129
 - large versus small scales, 125–128
 - physical picture, 124–125
 - polymer processing example, 129
 - velocity field, 128
 - viscous immiscible liquid mixing model, 156–159
- # Input analysis, process data
- adaptive resonance theory, 30–31
 - basis function, 14
 - classification of methods, 11, 14
 - cluster seeking, 28–29
 - definition, 4, 13
 - ellipsoidal basis function network, 30
 - latent variable representation, 10, 14
 - linear projection methods, 14–27
 - multiscale filtering
 - finite impulse response median hybrid filter, 19–20
 - steps in filtering, 22
 - temporal resolution, 19
 - threshold for filtering, 23
 - wavelet, 21–22
 - wavelet packet, 23–24
 - multivariate methods, 4–5, 10, 13, 24–27
 - nonlinear principle component analysis, 28
 - nonlinear projection methods, 27–32
 - principle component analysis
 - eigenvectors, 26–27
 - hierarchical blocking, 81
 - loadings, 24–25
 - multidimensional analysis, 27, 85
 - scores, 25
 - steps, 25
 - two principle component model example, 88–89
 - probabilistic methods, 4
 - process considerations in determining filter characteristics, 14
 - radial basis function network, 29–30
 - single-scale filtering
 - basis functions, 15
 - filter gain, 16
 - filter matching to response times, 17–18

- finite impulse response, 15–16, 18–19
 - infinite impulse response, 15–16, 18–19
 - linear phase filters, 19
 - phase shift, 16
 - univariate methods, 4, 13–19
- # Input–output analysis, process data
- back propagation networks, 38–39
 - basis functions
 - adaptive-shape basis functions, 13
 - fixed-shape basis functions, 12–13
 - classification and regression tree, 41–42
 - classification of methods, 11–12
 - linear projection methods, 33–40
 - multivariate adaptive regression splines, 42–43
 - nonlinear partial least squares, 37–38, 81
 - nonlinear principle component regression, 37
 - nonlinear projection methods, 40–41
 - ordinary least squares regression, 33–35, 52
 - overview, 4–5, 32–33
 - partial least squares, 36–37, 52, 85
 - partition-based methods, 41–43
 - principle component regression, 35–36
 - process output variable representation, 11
 - projection pursuit regression, 39–40
 - radial basis function network, 40–41

K

- KAM tube, *see* Kolmogorov–Arnold–Moser tube
- KBS, *see* Knowledge-based system
- Kenics static mixer, velocity field, 122
- Knowledge-based system (KBS)
 - applications, 66–67
 - decomposition of complex problems, 72, 93–94
 - digraph, 70
 - fault tree, 69–70
 - feed injection system example, 65–66
 - model-based methods, 68–69
 - overview, 44, 64–65
 - semantic networks, 67
 - tables, 65, 67, 70–71
- Kolmogorov–Arnold–Moser (KAM) tube, features, 116

M

- Multiscale filtering, input analysis of
 - process data
 - finite impulse response median hybrid filter, 19–20
 - steps in filtering, 22
 - temporal resolution, 19
 - threshold for filtering, 23
 - wavelet, 21–22
 - wavelet packet, 23–24
- Multivariate adaptive regression splines (MARS), input–output analysis of process data, 42–43

N

- Necking, *see* Breakup

O

- OLS, *see* Ordinary least squares
- Ordinary least squares (OLS), input–output analysis of process data, 33–35, 52

P

- Partial least squares (PLS)
 - input–output analysis of process data, 36–37, 52, 85
 - nonlinear partial least squares, 37–38, 81
- Partitioned-pipe mixer (PPM), features, 114, 116
- Pattern recognition, data analysis and interpretation, 2–3
- PCA, *see* Principle component analysis
- PCR, *see* Principle component regression
- Periodic operation, sulfur dioxide oxidation
 - applications, 206–207, 272–273
 - heat removal, 206
 - periodic air blowing of final stage of multistage catalytic converter
 - composition cycling results, 211–212
 - composition forcing, 216–217, 223
 - geographic distribution, 206–207
 - isothermal back-mixed reactor application, 217, 219–223

- mechanistic model, 215–216
- performance, 209–211, 272
- rate enhancement, 208–209
- temperature changes, 211–212, 272–273
- unsymmetrical cycling, 213–214
- periodic flow interruption in trickle-bed catalytic reactors
 - cycle period effects, 251–252
 - cycle split effects, 251–252
 - estimated oxidation rates, 255
 - geographic distribution, 206–207
 - intracycle gas removal, 270
 - liquid flow rate effects, 252–253
 - liquid loading, 253–254
- modeling and simulation
 - accuracy of models, 259–261
 - cycle split effects, 260
 - equations, 258
 - filling and draining steps, 256, 259
 - gas concentration estimation, 261
 - kinetics, 259
- physical mechanism, 269–272
- reactor design, 250
- segregation processes, 248–249
- space velocity, 251
- stack gas scrubbing
 - activated carbon performances, 263–264, 267, 269–270
 - advantages, 262–263
 - application, 273
 - bed depth estimation, 266–267
 - operating conditions, 264
 - pressure drop estimation, 267, 273
 - recommendations for improvement, 271–272
 - RTI–Waterloo process, 262, 273
 - wash liquid normality effects on removal, 264, 266
- temperature, 255–256, 270
- water role, 255
- periodic reversal of flow direction in single-stage converter
 - advantages, 247, 272
 - bench-scale unit design, 230, 232, 234
 - catalyst beds, 224–225
 - double contacting-double absorption process, 229–230
 - geographic distribution, 206–207, 223
 - modeling and simulations

Periodic operation (*Continued*)
 accuracy of models, 238–239
 boundary conditions, 238
 equations, 234–236
 heat recuperator effects, 242–243
 inlet sulfur dioxide concentration effects, 240, 242
 nonisothermal tubular reactor, 244–246
 operating problem identification, 243–244
 pseudo-homogeneous model, 236–237
 rate model, 238
 simplification, 237
 startup temperature jump, 243
 temperature, 239–240, 247
 performance of sulfuric acid plants, 225–227
 pilot-scale reactors, 227–229
 recuperator beds, 225
 sulfur dioxide concentration variation in feed, 225, 227
 temperature, 225
 PLS, *see* Partial least squares
 Polymer blend, advantages, 124
 Powder dispersion in liquids
 aggregation, *see* Aggregation
 fragmentation, *see* Fragmentation
 mixing optimization, 195, 198
 physical picture, 159–161
 stages, 160
 PPM, *see* Partitioned-pipe mixer
 Principle component analysis (PCA), input
 analysis of process data
 eigenvectors, 26–27
 hierarchical blocking, 81
 loadings, 24–25
 multidimensional analysis, 27, 85
 scores, 25
 steps, 25
 two principle component model example, 88–89
 Principle component regression (PCR)
 input–output analysis of process data, 35–36
 nonlinear principle component regression, 37
 Probability density function

approaches in process data interpretation, 56–58
 chaotic flow, 112–113
 Process data, *see* Data analysis; Data interpretation

Q

Q-statistics, process data analysis, 90

R

Radial basis function network (RBFN)
 clustering in process data interpretation, 61–62
 input analysis of process data, 29–30
 input–output analysis of process data, 40–41
 RBFN, *see* Radial basis function network
 Rupture, *see* Fragmentation

S

Shattering, *see* Fragmentation
 Single-scale filtering, input analysis of
 process data
 basis functions, 15
 filter gain, 16
 filter matching to response times, 17–18
 finite impulse response, 15–16, 18–19
 infinite impulse response, 15–16, 18–19
 linear phase filters, 19
 phase shift, 16
 Single screw extruder, improvement of
 mixing, 116
 Smoluchowski's equation, scaling solutions, 107, 183
 Stack scrubber, *see* Trickle-bed catalytic reactor
 Stokes equation, interface modeling for
 Newtonian fluids, 126–127
 Strain
 per period optimization in shear flows
 with periodic reorientation, 120–122
 shear zone dependence, 125
 Stretching
 chaotic flow islands, 113, 124
 distribution of values, 118, 120

- equations, 109–110
 - flow classification, 131–132
 - low-viscosity-ratio elongated drops, 137–138
 - preconditions, 125
 - quantitative estimation, 122
 - viscous immiscible liquid mixing model, 157
 - Sulfur dioxide oxidation
 - applications, 206–207, 272–273
 - heat removal, 206
 - periodic air blowing of final stage of multistage catalytic converter
 - composition cycling results, 211–212
 - composition forcing, 216–217, 223
 - geographic distribution, 206–207
 - isothermal back-mixed reactor
 - application, 217, 219–223
 - mechanistic model, 215–216
 - performance, 209–211, 272
 - rate enhancement, 208–209
 - temperature changes, 211–212, 272–273
 - unsymmetrical cycling, 213–214
 - periodic flow interruption in trickle-bed catalytic reactors
 - cycle period effects, 251–252
 - cycle split effects, 251–252
 - estimated oxidation rates, 255
 - geographic distribution, 206–207
 - intracycle gas removal, 270
 - liquid flow rate effects, 252–253
 - liquid loading, 253–254
 - modeling and simulation
 - accuracy of models, 259–261
 - cycle split effects, 260
 - equations, 258
 - filling and draining steps, 256, 259
 - gas concentration estimation, 261
 - kinetics, 259
 - physical mechanism, 269–272
 - reactor design, 250
 - segregation processes, 248–249
 - space velocity, 251
 - stack gas scrubbing
 - activated carbon performances, 263–264, 267, 269–270
 - advantages, 262–263
 - application, 273
 - bed depth estimation, 266–267
 - operating conditions, 264
 - pressure drop estimation, 267, 273
 - recommendations for improvement, 271–272
 - RTI–Waterloo process, 262, 273
 - wash liquid normality effects on removal, 264, 266
 - temperature, 255–256, 270
 - water role, 255
 - periodic reversal of flow direction in single-stage converter
 - advantages, 247, 272
 - bench-scale unit design, 230, 232, 234
 - catalyst beds, 224–225
 - double contacting-double absorption process, 229–230
 - geographic distribution, 206–207, 223
 - modeling and simulations
 - accuracy of models, 238–239
 - boundary conditions, 238
 - equations, 234–236
 - heat recuperator effects, 242–243
 - inlet sulfur dioxide concentration effects, 240, 242
 - nonisothermal tubular reactor, 244–246
 - operating problem identification, 243–244
 - pseudo-homogeneous model, 236–237
 - rate model, 238
 - simplification, 237
 - startup temperature jump, 243
 - temperature, 239–240, 247
 - performance of sulfuric acid plants, 225–227
 - pilot-scale reactors, 227–229
 - recuperator beds, 225
 - sulfur dioxide concentration variation in feed, 225, 227
 - temperature, 225
- T**
- Tipstreaming, *see* Breakup
 - Trickle-bed catalytic reactor, periodic

Trickle-bed catalytic reactor (*Continued*)

- flow interruption in sulfur dioxide oxidation

- cycle period effects, 251–252

- cycle split effects, 251–252

- estimated oxidation rates, 255

- geographic distribution, 206–207

- heat removal, 206

- intracycle gas removal, 270

- liquid flow rate effects, 252–253

- liquid loading, 253–254

- modeling and simulation

- accuracy of models, 259–261

- cycle split effects, 260

- equations, 258

- filling and draining steps, 256, 259

- gas concentration estimation, 261

- kinetics, 259

- physical mechanism, 269–272

- reactor design, 250

- segregation processes, 248–249

- space velocity, 251

- stack gas scrubbing

- activated carbon performances, 263–264, 267, 269–270

- advantages, 262–263

- application, 273

- bed depth estimation, 266–267

- operating conditions, 264

- pressure drop estimation, 267, 273
- recommendations for improvement, 271–272

- RTI–Waterloo process, 262, 273

- wash liquid normality effects on removal, 264, 266

- temperature, 255–256, 270

- water role, 255

V

VILM, *see* Viscous immiscible liquid mixing model

Viscoelastic fluid, mixing, 116–118, 124

Viscous immiscible liquid mixing model (VILM)

- drop size distribution, 157–158

- physical aspects, 156

- stretching distributions, 157

- viscosity ratio, dispersed phase size dependence, 158–159

Viscous mixing, overview, 107–108

Vortex mixing flow, characteristics, 110

W

Wavelet, *see* Multiscale filtering