Ref.660.2 ADV V.37

ABACUS, 59

ADAC Forte, 154 Adhesion strength, measurement of of bacteria, 72-73 food fouling, 75 Advantose[™] 100, 63, 64, 65 AFM. See Atomic force microscopy (AFM) Algebraic reconstruction techniques (ART), 182 Alginate, 58 Alginate-chitosan microcapsules, 58-59 Ambient air studies, in automotive soot investigations, 260-262 Animal cells, in suspension culture, 51-53 Ar laser, 94, 138 Aspergillus nidulans, 56 Atomic force microscopy (AFM), 33-35, 54, 56, 70-71, 73, 74 Automotive soot investigations ambient air studies, 260-262 inside and outside the car, 261-262 LII applications, 251-262 LII exhaust gas sensor, 251-254 raw exhaust gas measurements, 254-260 Awet. See Liquid phase (Awet) Axial dispersion coefficient, D, 165 Bacillus subtilis, 37, 55 "Back-to-back" y-rays, 151 Bacterial cells, 54-55 adhesion strength of, measurement of, 72 - 73Barcroft™ CS90 calcium carbonate, 63 Biocompatible particles, 58-59. See also Micromanipulation, in mechanical characterisation of single particles

Biological particles. See also Micromanipulation, in mechanical characterisation of single particles animal cells, in suspension culture, 51-53 chondrocytes, 53-54 filamentous microorganisms, 56 plant cells, 56-57 yeast and bacterial cells, 54-55 Biomass and biofilm formation, fouling of surfaces by, 72-74 Birmingham positron camera, 154, 171 Boltzmann integral expression, 43 BP's Hull Research and Technology Centre, 173 Brunauer-Emmett-Teller (BET) analysis, 240-241 Bubbly flow, in gas-liquid two-fluid flows measurement, 121, 125-136 Calcium alginate microspheres, 58, 59 Calcium-shellac microsphere, 59 CARPT. See Computer-automated radioactive particle tracking technique (CARPT) Cartesian coordinates, 18 Cell poking technique, 33-35 CFB. See Circulating fluidised beds (CFB) Chitosan, 58, 59 Chondrocytes, 53-54 Chondrons, defined, 53 CIP. See Cleaning-in-place (CIP) Circulating fluidised beds (CFB), 156, 159 - 160ECT applications in, 186-190 Cleaning-in-place (CIP), 74

Coherent anti-stokes Raman scattering (CARS) thermometry, 236

Compression testing, by micromanipulation. See Diametrical compression Computed tomography (CT), 182 Computer-automated radioactive particle tracking technique (CARPT), 150-151 Confocal µ-PIV technique, 104-105, 120 Continuously regeneration trap (CRT) filter system, 258 Continuous wave (CW) lasers, 94-95 Core/shell structure of microparticles, models for, 44-51 Coriolis flow meter, 11-12 Correlation analysis for gas-liquid interface heights, 15-16 Correlation coefficient, defined, 15 Cross-correlation analysis, for PIV technique, 97-98 CTI ECAT931/08, 171-172 ⁶¹Cu (half-life 3.4 h), 154 DCPD. See Dicyclopentadiene (DCPD) Defocusing concepts, 111 Defocusing particle image velocimetry (DPIV) technique, 111-112 DEM. See Discrete element modelling (DEM) Diametrical compression, 37-51 experimental setup, 37-40 microcapsules and, 65-67 of single particles, mathematical modelling of Hertz model, 40-41 microparticles with core/shell structure, models of, 44-51 Tatara analysis, 41-42 viscoelastic model, 42-44 of two-week-old suspension-cultured tomato cells, 57 Dicyclopentadiene (DCPD), 67 Dielectric particle, optical trapping of, 35-36 Dipalmitoyl phosphatidyl choline (DPPC), 70 Discrete element modelling (DEM), 164 Disc-shearing device, 72–73 Dispersion of particle pulse in gas-solid fluidized beds, PET applications in, 212-213 Dispersion time, defined, 167 DLVO theory, 68

Doppler velocimetry, 2-3 laser, 2 ultrasonic, 3 DPPC. See Dipalmitoyl phosphatidyl choline (DPPC) Dual-plane PIV, 117-118 Dynamic light scattering (DLS), 224, 262 Dynamic PIV, 115 Elastic membrane model, 44-47, 57 Electrical capacitance tomography (ECT), 180--196 applications, 186-196 circulating fluidized beds (CFB), 186-190 hydrodynamic behaviors in bubble and slurry bubble columns, 191-196 pneumatic solid conveying, 190-191 principle of, 183-186 Electrical capacitance volume tomography (ECVT), 192-194, 196-197, 215 Electrical impedance tomography (EIT), 198, 200-202 strategies employed in, 200-202 Electrical magnetic tomography (EMT), 181 Electrical resistance tomography (ERT), 196-209 applications, 204-209 high-speed flow imaging in slurry conveying, 205-207 hydrocyclone flow visualization and comparison with computational fluid dynamics, 204-205 visualization of dispersions in an oscillatory baffled reactor, 207-209 principle of, 198-203 Electromagnetic flow meters, 11-12 Electron microscopy, 76 Energy balance, determination and LII signal, 225-228 Environmental scanning electron microscope (ESEM), 76-77 EPS. See Exopolysaccharides (EPS) Escherichia coli, 55 ESEM. See Environmental scanning electron microscope (ESEM)

Eudragit[®] L100-55, 62-65 Eudragit microparticles, 39 Eudragit[®] S100, 63 3D Euler–Lagrangian hardsphere discrete particle model (DPM), 160 Excipients, pharmaceutical, 61-64 Exopolysaccharides (EPS), 72 ¹⁸F (half-life 110 min), 153–154 Filamentous microorganisms, 56 Flame investigations, by LII, 236-237 Fluidised beds, PEPT used in circulating fluidised beds (CFBs), 159-160 Fluidized beds, PEPT used in computational models, validation of, 160 - 162motion close to surfaces, 158-159 solids motion studies, 156-158 Food fouling deposits, 74–75 Force spectroscopy, 34 Fouling, of surfaces biomass and biofilms, 72-74 food fouling deposits, 74-75 Four-pulse ultrasound wave, at gas-liquid interface, 7 Free-surface flow, in gas-liquid two-fluid flows measurement, 121-125 Furnace black reactor, 242-245 Fusarium graminearum, 56 ⁶⁶Ga (9.3 h), 154 Gas-liquid interface four-pulse ultrasound wave at, reflected, 7 liquid velocity and experimental approach, 6-10 experimental setup, 4-5 proposed experimental method, validation of, 10-11 peak ultrasound echo intensity and, 3, experimental approach, validation of, 18–24 experimental setup, 12-13 method, experimental, 13-18 Gas-liquid two-fluid flows measurement using PIV technique, 121-137

bubbly flow, 125-136

- free-surface flow, 121-125
- gas-liquid two-phase flows in microchannels, 136-137

Gas-liquid two-phase flows in microchannels, in gas-liquid two-fluid flows measurement, 136–137

- γ-ray tomography (GRT), 181 Green strain, defined, 49
- Hencky/true strain, defined, 49–50
- He–Ne laser, 94
- Hertz equation, 41
- Hertz model, 40-41
- High-speed flow imaging in slurry conveying, ERT applications in, 205–207
- Holographic particle image velocimetry (HPIV) technique, 109–111
- Hooke's law strain energy function, 45, 49
- Hot wall reactor, 249-251
- Hot-wire anemometry, 2
- Hydrocyclone flow visualization and comparison with computational fluid dynamics, ERT applications in, 204–205
- Hydrodynamic behaviors in bubble and slurry bubble columns, ECT applications in, 191–196
- Imaging tomography, 2
- Instantaneous shear modulus (G₀), 43
- Ion-exchange resin particle, 38-39
- Iterative linear back projection (ILBP), 185–187

JKR theory, 69 Jurket T lymphomas cells, 35

Kelvin-Voigt element, 42

Lactose, particle–surface interactions of AFM for, 70 Laplacian filter, 7–8 Lardner and Pujara's model, 67 Laser Doppler velocimetry, 2 Laser-induced fluorescence (LIF) technique, 92, 119, 121, 127–137, 139–140

Laser-induced incandescence (LII), 224 applications, 237-265 automotive soot investigations, 251-262 nanoparticle production processes control, 237-251 particle suspensions, 262-265 flame investigations, 236-237 signal and determination of energy balance, 225-228 primary particle size and its distribution, 228-236 Laser-Induced Soot Analyzer (Ll²SA), 253, 255 Laser trapping, 68–70 Laser tweezers. See Optical trapping method Laser vaporization reactor (LVR), 246-249 LII exhaust gas sensor, 251-254 Linear back projection (LBP) technique, 185-187, 203 Linear forward projection (LFP) technique, 184 "Liquid-drop" model, 44 Liquid-liquid two-fluid flows measurement, using PIV technique, 119-121 Liquid phase (A_{wet}), calculation of portion of pipe occupied by, 16-18 Liquid velocity gas-liquid interface inferred from experimental approach, 6-10 experimental setup, 4-5 proposed experimental method, validation of, 10-11 Loading and unloading curves, 39-40 Local-field correlation particle image velocimetry (LFCPIV) method, 99 Long-term shear modulus (G_{∞}) , 43 Lycopersicon esculentum, 56 Markov chain Monte Carlo (MCMC) method, 202 MATLAB ode45 solver, 50 Maxwell model, 42 ME. See Mixer effectiveness (ME) Mean von Mises stress, 54

Mechanical characterisation of single particles, micromanipulation in. *See* Micromanipulation, in mechanical characterisation of single particles Mechanotransduction, 53 Melamine formaldehyde (MF) microcapsules, 67 microparticles, 71 Metal and metal oxides production reactors, 246-251 hot wall reactor, 249-251 laser vaporization reactor, 246-249 MF. See Melamine formaldehyde (MF) Microcapsules, 65-67 Micromanipulation, in mechanical characterisation of single particles, 29-85 status and applications biocompatible particles, 58-59 biological particles, 51-57 fouling deposits on surfaces, 72-75 non-biological particles, 59-67 particle adhesion to surface, 70-72 particle-particle adhesion, 68-70 sub-micron/nanoparticles, nanomanipulation of, 75-77 techniques for cell poking and atomic force microscopy (AFM), 33-35 diametrical compression. See Diametrical compression micropipette aspiration, 32-33 optical trapping, 35-37 pressure probe, 31-32 Micropipette aspiration, 32-33, 53, 68 Microspheres, 59-65 chromatographic resins, 60-61 pharmaceutical excipients, 61-65 Mixer effectiveness (ME), 167 Mooney–Rivlin model, 45

Nanomanipulation, of sub-micron/ nanoparticles, 75–77 Nanoparticle production processes control, 237–251 furnace black reactor, 242–245 LII applications to, 237–251 metal and metal oxides production reactors, 246–251 hot wall reactor, 249–251 laser vaporization reactor, 246–249 research plasma reactor, 237–242 Nd:YAG lasers, 94, 103–104, 115, 117, 136, 238–239, 249, 253, 263 Neo-Hookean equations, 67 Neural network multi-criterion image reconstruction technique (NN-MOIRT), 185–188

Newton-Raphson method (NRM), 203

N-methylmorpholine-N-oxide (NMMO), 71

NMMO. See N-methylmorpholine-Noxide (NMMO)

Non-biological particles. *See also* Micromanipulation, in mechanical characterisation of single particles microcapsules, 65–67

microspheres, 60–61 chromatographic resins, 59–61 pharmaceutical excipients, 61–64

Optical trapping method, 35–37 Optimization reconstruction techniques (ORT), 182

Orthogonal-plane PIV technique, 118

"Packet model", 158

- Particle adhesion, to surface, 70-72
- Particle collision dynamics, 160

Particle image accelerometry technique (PIA), 139

Particle image velocimetry (PIV) technique, 2

fundamentals, 90–102, 113 analysis, 95–101 cross-correlation analysis, 97–98 error elimination and accuracy

improvement, 100-101

illumination and image recording, 92, 94–95

post-processing of velocity vectors, 101-102

resolution improvement, 98–100 seeding flow, 91–93

multiphase flow measurement using, 118-140

gas-liquid two-fluid flows, 90, 92, 119–137

liquid-liquid two-fluid flows, 119-121

particle-laden multiphase flows, 137–140

seeding particles used for, 93 types, 102–118

2D-2C PIV techniques, 103–105 2D-3C PIV techniques, 105–108 3D-3C PIV techniques, 109–115

dual-plane PIV, 117-118 dynamic PIV, 94-95, 103, 109, 115 orthogonal-plane PIV technique, 118 scanning PIV, 115-116 Particle-laden multiphase flows measurement, using PIV technique, 137 - 139Particle-particle adhesion, 68-70 Particle suspensions, LII applications to, 262-265 Particle tracking velocimetry (PTV) algorithms, 98, 107, 112, 133-135, 140 PCM. See Pericellular matrix (PCM) Peak-locking error, 100-101 Peak ultrasound echo intensity gas-liquid interface inferred from, 11 experimental approach, validation of, 18-24 experimental setup, 12-13 method, experimental, 13-18 PEPT. See Positron emission particle tracking (PEPT) Pericellular matrix (PCM), 53 PET. See Positron emission tomography (PET) Piezoelectric scanner, 34 Piezoelectric stack, for compression method, 38 PIV. See Particle image velocimetry (PIV) 2D-2C PIV techniques, 94, 103-105 macro scale, 103 micro scale, 103-105 2D-3C PIV techniques, 105-108 macro scale, 105-108 micro scale, 108 3D-3C PIV techniques, 109-114 DPIV technique, 111-112 HPIV technique, 109-111, 114 macro scale, 109-114 micro scale, 114 TPIV technique, 112-114 Plane stress, defined, 45 Plant cells, 56-57 Plasmodium falciparum, 52 Pluronic F68, 52 PMMA nanoparticles. See Polymethylmethacrylate (PMMA) nanoparticles

Pneumatic solid conveying, ECT applications in, 190–191

Poisson ratio, 33 Polymethylmethacrylate (PMMA) nanoparticles, 76 Polyurethane microcapsules, 67 Portable PEPT, 168-174. See also Positron emission particle tracking (PEPT) Positron emission particle tracking (PEPT), 151-153 applications of, 169 fluidised beds, 156-160 rotating drums and kilns, 162-163 solids mixing, 163-168 detectors, 154-155 and PET, difference between, 151 portable, 168, 171-173 positron-emitting tracers, 153-154 principles of, 151-152 technique development, 155 Positron emission tomography (PET), 180-182, 209-215 applications, 211-215 dispersion of particle pulse in gassolid fluidized beds, 212-214 slurry mixtures in stirred tanks, 211-212 visualization of multi-phase fluids through sudden expansions, 213-214 principle, 209-211 Positron emission tomography (PET) and PEPT, difference between, 151 Positron-emitting tracers, 153-154 Positron Imaging Centre at Birmingham, 154 Pressure probe, 31-32, 57 Primary particle size and its distribution, LII signal and determination of, 228-236 Pseudomonas fluorescens, 73 Pulsed lasers, 90, 91, 94, 115 Radioactive particle tracking (RPT), 181 Raman spectroscopy, 36 Ramp correction factor (RCFi), 43 Raw exhaust gas measurements, in automotive soot investigations, 254-260 Rayleigh-Debye-Gans (RDG) approach, 236 RBCs. See Red blood cells (RBCs) RCFi. See Ramp correction factor (RCFi) Red blood cells (RBCs), 32 stretching of, using optical trapping method, 36 Research plasma reactor, 237-242 Residence time, defined, 158-159 Resins, chromatographic, 60-61 Rotating drums and kilns, 162-163 Runge-Kutta method, 50 Saccharomyces cerevisiae, 35, 54-55 Saccharopolyspora erythraea, 56 Scanners, for medical PET, 155 Scanning electron microscopes (SEMs), 76 Scanning mobility particle sizers (SMPS), 224 Scanning PIV, 115-116 SEMs. See Scanning electron microscopes (SEMs) Sensitivity conjugate gradients (SCG) method, 203 Shadow image technique (SIT), 127-136, 140 SIRT, 186-187 Skalak-Tozeren-Zarda-Chien (STZC) material relationship, 45 Slurry mixtures in stirred tanks, PET applications in, 211-212 Sobel filter, 8, 9 Solids mixing, PEPT and PET used in, 163 - 168Sound, use of, in science and technology, 2 Speckle correlation velocimetry, 3 Standard stirred tank reactors (STR), 207, 211-212, 216 Starlac[™], 63 Stereoscopic µ-PIV technique, 108 Stereoscopic PIV system, 106-107 Strain energy, defined, 45 Stretch ratios, defined, 45 STZC. See Skalak-Tozeren-Zarda-Chien (STZC) Sub-micron/nanoparticles, nanomanipulation of, 75-77 Tapered element oscillating microbalance (TEOM), 261 Tatara analysis, 41-42, 61 Time-resolved laser-induced incandescence (TIRE-LII), 223-266 Tomato. See Lycopersicon esculentum

- Tomographic particle image velocimetry (TPIV) technique, 112–115
- 4V transistor-transistor logic signal, 13 Transmission electron microscopy

(TEM), 224 Turgor (hydrostatic) pressures, within cells, 32

- Ultrasonic Doppler velocimetry, 3 Ultrasonic velocity profiler (UVP) measurements, 1, 2, 4. See also Gas-liquid interface Ultrasound echo intensity, 10-11, 13-15,
- 20 Ultrasound tomography (UST), 205
- Ultrasound transducer arrangement, 14
- Urea-formaldehyde microcapsules, 67
- UVP-DUO systems, 2, 7, 12-13
- UVP measurements. See Ultrasonic velocity profiler (UVP) measurements

Video microscopy, 32 Viscoelastic model, 42–44, 53, 59

- Visualization of dispersions in an oscillatory baffled reactor, ERT applications in, 207–209 Visualization of multi-phase fluids through sudden expansions, PET applications in, 214
- V-mixer, 163
- Volumetric elastic modulus, 32
- We. See Weber number (We)
- Weber number (We), 6
- Window displacement iterative multigrid (WIDIM) interrogation method, 99
- XPS. See X-ray photoelectron spectroscopy (XPS)
 X-ray photoelectron spectroscopy (XPS), 72
- Yeast. See Saccharomyces cerevisiae Young's modulus, 33, 35, 53–54

Ref.660.2 ADV V.38



Note: The letters 'f' and 't' following locators refer to figures and tables respectively.

Acid-catalyzed microreactions aldehyde protection as its dimethyl acetal, 140f continuous flow thioacetalizations, 141t continuous flow thioketalizations using EOF, 142t enantioselective synthesis in microreactor, 143f Strecker reaction, PS-RuCl₃/PS-Sc(OTf)₂, 144t synthesis of dimethyl acetals under continuous flow, 140t N-Acyl oxazolidinone, alkylation of, 117, 117f Adsorbed molecules, control of activity adsorbing proteins, orientation experimental study, SIMS/atomic force microscopy, 92 theoretical study, molecular/ continuum models, 91-92 external electric field effects, 92-93 NEMCA effect, mechanism, 94-95 PABA, potential-dependent orientation effect, 91 Adsorption-desorption by electrical fields adsorption control on surface, principles FET configuration by gate potential, 89 field-effect control, 89 interaction of gases with catalyst surfaces FEM, 86 FIM, 86 interaction of CO and O2 with gold, 86-87, 87f 'microorganism' as a microreactor enzymes immobilization strategies, 88

heat application to enzymes, effects, 88-89 MOF, separation of gas mixtures, 87-88 physical/chemical field effects, 85-86 protein adsorption (reversible and nonspecific), 89-90 protein microarrays, development of, 90-91 Alkylation of N-acyl oxazolidinone, 117, 117f Aminonaphthalene derivative, synthesis of, 181, 182f α-Aminophosphonates synthesis, Kabachnick-Fields reaction, 111, 111f Amphibole, 225, 226f Applications of microplasma reactors chemical synthesis ammonia/CO2 decomposition, use of MHCD, 57-58 fabricated plastic microreactors, study (Anderson), 61 hydroxylation of benzene and toluene by DBD, 58-59, 58f oxidative conversion of C1-C3 alkanes by DBD, 59-60, 59f partial oxidation of methane, microreactor setup, 56-57, 57f environmental applications CO2 decomposition by plasma reactors, 54-55, 55f nanostructures as electrodes, 55, 56f tetrafluoromethane decomposition by microreactors, 54, 54f VOCs decomposition by microplasma reactors, 53-54, 53f nanostructure synthesis CNF growth, 51

Applications of microplasma reactors (Continued) microplasma in capillary/Pyrex chip, 52, 53f microreactor/catalyst coating/ microplasma treatment, 51, 52f synthesis of Fe/Ni catalyst particles (Chiang & Sankaran), 49 synthesis of MoO2 nanoparticles with UHF, 50-51, 50f synthesis of photoluminescent silicon nanocrystals by VHF, 49, 50f synthesis of silicon nanoparticles (Sankaran), 48, 49f UHF technique in MWCNTs, 51 plasma generation in liquid/at liquid interface, 61-67. See also Electrohydraulic discharge Arylation of octafluorocyclopentene, 178t Asbestos fibers, types amphibole, 225, 226f serpentine, 225, 226f Atmospheric pressure microplasmas classification factors, 41, 42 DBDs and configurations, 43-44, 44f DC glow discharges, 42, 43t field emission from tip electrodes, 45 - 48MHCDs, 44-45, 44f microcavity discharges, 45, 45f examples arc discharges, 39 corona discharge, 39 DBD, 39 high-pressure plasmas, 42. See also Microplasma nonequilibrium atmospheric pressure plasma applications, 41-42 plasma state, 41 plasma temperature, 41 Automated microreactors application in nanotoxicology asbestos fibers, types, 225, 226f libraries of RMs, study, 227 "scale-out" process, benefits, 228 toxicity, influencing factors, 227

effectiveness of automation process, criteria, 211 ideal behavior, 211f key features, 211-212 MAUFs/SAUFs, 220 minimization routines design, conditions, 213-214 optimization techniques. See Noise-free optimization, technique nanoparticles formation with desired properties, set up, 212f parts of decision-making software, 211 online detectors, 211 physical machinery, 211 search process for optimization routines, phases global searching, 222 local searching, 222 utility function, 212, 213f Band-edge emission, 209, 209f Barton reaction (nitrite photolysis), 188. 190t Base-promoted microreactions, 136-139 AO-DMAP as catalyst for acylation of 2° alcohols, 138, 138f base-catalyzed Knoevenagel condensation, 136, 136f derivatization of PGMA polymer, model reaction, 138, 138f synthesis of (E)-ethyl-2-cyano-3phenylacrylate, model reaction, 137, 137f synthesis of thiazoles and imidazoles, 138-139, 139f, 139t α , β -unsaturated compounds synthesis by silica-supported base, 137t Bead-packed microchannels, 11-12, 12f (4-Benzyloxynaphthalen-2-yl)-carbamic acid tert-butyl ester, microreactions used, 182, 183f **Biocatalysis reactions** biocatalytic hydrolysis of 2-phenoxymethyloxirane, 152f continuous flow ester hydrolysis using His₆-tag BsubpNBE, 157f

continuous flow optical resolution of acetyl-D,L-phenylalanine, 156f enzymatic synthesis of L-lactate, 157f immobilization of Hiss-tagged proteins, 156f PDMS microreactor, reactions conducted in, 154f-155f Biphasic fluorination, 122 "Black-box" automated reactors, 211 Black-box technique. See Simplex method Block copolymers, 132 BOLSIG+ software, 60 Bond (Bo) number, 15 Bromination reactions, 115, 115f CAD. See Computer-aided design (CAD) Capillarity restricted modification (CARM) method, 27, 29f Carbamates, exothermic synthesis, 176f Carbon nanofiber (CNF), 51 Carbon nanotubes (CNTs), 47. See also Multiwalled carbon nanotubes (MWCNTs) CARM method. See Capillarity restricted modification (CARM) method Catalyst incorporation into microreactors acid-catalyzed microreactions aldehyde protection as its dimethyl acetal, 140f continuous flow thioacetalizations, 141t continuous flow thioketalizations using EOF, 142t enantioselective synthesis in microreactor, 143f Strecker reaction, PS-RuCl₃/PS-Sc (OTf)₂, 144t synthesis of dimethyl acetals, continuous flow, 140t base-promoted microreactions, 136-139 AO-DMAP as catalyst for acylation of 2° alcohols, 138, 138f base-catalyzed Knoevenagel condensation, 136, 136f derivatization of a PGMA polymer, model reaction, 138, 138f synthesis of (E)-ethyl-2-cyano-3phenylacrylate, model reaction, 137, 137f

synthesis of thiazoles and imidazoles, 138-139, 139f, 139t α , β -unsaturated compounds synthesis by silica-supported base, 137t biocatalysis continuous flow ester hydrolysis using His₆-tag BsubpNBE, 157f continuous flow optical resolution of acetyl-D,L-phenylalanine, 156f enzymatic synthesis of L-lactate, 157f hydrolysis of 2-phenoxymethyloxirane, 152f immobilization of His6-tagged proteins, 156f PDMS microreactor, reactions conducted in, 154f-155f metal-catalyzed reactions, 145-148 continuous flow Heck-Mizoriki reaction, 146t continuous flow Suzuki-Miyaura reaction, 145t kinetic resolution of rac-4-hdroxy-1butene oxide, 146, 146f Suzuki-Miyaura coupling reactions, 147t multiple catalyst systems multistep synthesis of an α,β -unsaturated compound, 149f polymer-assisted derivatization of steroid, 149f solid-supported reagents in single pressure-driven flow reactor, 150f synthesis of 2-(benzyloxy) tetrahydropyran, 151t "Cation flow" process, 68 CdSe nanoparticles, production of Peng's method, 208 reactor design, 208f TEM image/emission spectrum/ wavelenghts, 208-209, 209f temperature dependence of emission spectra of, 209, 210f total flow-rate dependence of emission spectra of, 209, 210f CFCP. See Continuous-flow chemical processing (CFCP)

Chemical reactions, electrokinetic control of electrophoresis/electroosmosis, 72-77 EWOD, 81-82 positioning/trapping of particles/ molecules, 77-81 special effects electric swing adsorption, 83-84 electric wind, 82-83 electrospray, 84-85 pulsed electric fields, 84 Chemical surface modification methods Beebe's group study by multiphase laminar microflows, 26, 26f UV photopatterning method, 26-27, 28f Kitamori's group study CARM method, 27, 29f Chemical synthesis in microplasma reactors ammonia/CO₂ decomposition, use of MHCD, 57-58 fabricated plastic microreactors, study (Anderson), 61 hydroxylation of benzene and toluene by DBD, 58-59, 58f oxidative conversion of C1-C3 alkanes by DBD, 59-60, 59f partial oxidation of methane, microreactor setup, 56-57, 57f Chemkin plasma reactor model, 60 CNF. See Carbon nanofiber (CNF) CNTs. See Carbon nanotubes (CNTs) Cold plasma processing, 59 Computer-aided design (CAD), 11 Continuous-flow chemical processing (CFCP), 1-33 Conventional emission spectroscopy techniques, 65 Corona discharge application, 39 configurations, 63, 63f gas-liquid pulsed corona discharge reactor, applications aqueous electrode chip design, 65f conventional emission spectroscopy techniques, 65 degradation of 4-chlorophenol in water, 64 electrolyte as a cathode discharge, 65

electrons injected into liquid by nanowires, 66-67 flue gas desulfurization, 64 liquid paraffin in glow-discharge plasma, 64-65 segmented flow patterns with DBD, 66, 66f DBD. See Dielectric barrier discharge (DBD) DC glow discharges, 42, 43f Decomposition of enolate, batch conditions, 117-118, 118f Dehydration of β-hydroxyketones, 112, 112f MRT/batch flow approach, 112 DEP. See Dielectrophoresis (DEP) Deprotonation of styrene oxide, reaction products, 131t Derjaguin-Landau-Verwey-Overbeek theory, 92 Dielectric barrier discharge (DBD), 39, 43-44, 44f Dielectrophoresis (DEP), 39 2,4-Dihydrobenzoic acid from resorcinol, Kolbe-Schmitt synthesis, 112, 112f in microreactor/batch reactor, 113 Domino reactions (Fernandez-Suarez), 105, 105f Duocarmycin synthesis, 181f Efaproxiral synthesis, batch/flow methodology, 180f Electric swing adsorption, 83-84 Electrochemical microreactors carbocations for nucleophilic reactions, 70 cofactor generation DNA restriction schemes, 72 immobilization of enzymes, 71 microfluidic fuel cell, 68 microreactor coupling to separation methods, 70-71 electrochemistry at static triple-phase boundaries, 69 electrosynthesis in microfluidic system, purpose, 67-68 'supporting electrolyte' elimination two-phase flow with NOP, 69 Electrochemistry, 38 Electrohydraulic discharge

corona discharge. See Corona discharge pulsed arc discharge, 63 Electromigration dispersion, 74 Electronic control of reactions at surfaces adsorption-desorption by electrical fields, 85-91 control of activity of adsorbed molecules, 91-95 Electroosmosis, 39, 72-77 Electrophoresis, 39, 72 Electrophoretically mediated microanalysis, 75 Electrospray, 84-85 Electrowetting-on-dielectric (EWOD), 39, 81 - 82Enhanced reaction control by MRT acylation of primary amines deuterium labels incorporation, method, 110, 110f Domino reactions in a soda-lime microreactor, 105, 105f ester synthesis in EOF-based microreactor, 109, 109f synthesis of 1,2-azoles by EOF, 105-106, 106t synthesis of chromenones, 106-107, 107f, 108t 3-amino-4-(arylamino)-1H-isochromen-1-ones, model reaction, 108f 1H-isochromeno[3,4-d]imidazol-5-ones synthesis, 109t Environmental applications of microplasma reactors CO2 decomposition by plasma reactors, 54-55.55f nanostructures as electrodes, 55, 56f tetrafluoromethane decomposition by microreactors, 54, 54f VOCs decomposition by microplasma reactors, 53-54, 53f EWOD. See Electrowetting-on-dielectric (EWOD) Exothermic synthesis of carbamates, 176f Extended nanospace, 4 Fanetizole, continuous flow synthesis, 175f FEM. See Field emission microscopy (FEM)

FEM. See Field emission microscopy (FEM Fenchone/2-bromopyridine, one-step coupling

model reaction, 129, 129f optimization strategy, 130t FET. See Field-effect transistor (FET) Field-effect flow control principle, 89 Field-effect transistor (FET), 89 Field emission, definition, 46 Field emission from tip electrodes current determination, Fowler-Nordheim equation, 46 gate electrode, features, 47-48 nanowires, applications, 47 Paschen curve, 45, 46f Spindt type emitter, 47 with integrated gate electrode, 47f Field emission microscopy (FEM), 86 Field-induced adsorption/desorption. See Adsorption-desorption by electrical fields Field ion microscopy (FIM), 86 FIM. See Field ion microscopy (FIM) Fluorination of β -diketoester, 122, 122f Fluorinations in organic molecules (Miyake and Kitazume) 122-127 Horner-Wadsworth-Emmons reaction. 123, 126f Michael addition reaction, 123, 126f Formation of nanoparticles continuous-flow synthesis of ZnS-coated CdSe composite particles, 203, 204f in microfluidic device absence of turbulence, advantage, 202 benefits, 198-199 in chemical synthesis, features, 199 choice of solvent, criteria, 202-203 fabrication materials, 200 lab-on-a-chip, 199 used for DNA processing, 200f using wet lithography, 199f y-shaped microfluidic device, design, 201, 201f nucleation stage/growth phase, 197, 198f one-pot synthesis of II-VI nanoparticles, findings, 206 sulfur colloids, formation of, 197 "supersaturation"/"critical" concentration, 197 synthesis of anisotropic particles (Millman), 206

Formation of nanoparticles (Continued) synthesis of CdSe nanoparticles, 203 synthesis of CdSe/ZnS and CdS/ZnS nanoparticles, 205, 205f synthesis of high-quality CdSe quantum dots, 206, 207f synthesis of ZnS/CdSe/ZnS QDQW, 203-204 Ostwald ripening of cores, effects, 204 "top-down"/"bottom-up" approach, 196 Fowler-Nordheim equation, 46 Gas chromatography-mass spectrometry (GC-MS), 13, 109 Gate electrode, features, 47-48 GC--MS. See Gas chromatography--mass spectrometry (GC-MS) Grossamide synthesis, 187f Halide displacement reaction, 115, 115f Heterogeneous immunoassay integration of ELISA with microchip bead-packed microchannels, use of, 11-12, 12f His₆-tagged proteins benzoin/cross-benzoin reaction, 156f immobilization of, 156f HIV-1 RTI analog, continuous flow synthesis, 186f Horner-Wadsworth-Emmons reaction, 123, 126, 126f comparison of stereoselectivities in batch/ microreactor, 126, 127t Hydraulic diameter, 16 Hydrolysis free O-acylation of alcohols, 114, 114f 6-Hydroxybuspirone, synthesis of, 184f Industrial applications of MRT arylation of octafluorocyclopentene, 178t (4-benzyloxynaphthalen-2-yl)-carbamic acid tert-butyl ester, microreactions used, 182, 183f

continuous flow synthesis of a HIV-1 RTI analog, 186f continuous flow synthesis of fanetizole, 175f

continuous flow synthesis of pristane, 184-185, 185f continuous flow synthesis of rimonabant, 180f continuous flow synthesis of spiro lactone derivative, 174f, 175t conversion of nitrite to oxime, 189, 189f exothermic synthesis of carbamates, 176f flow-assisted synthesis of (+)oxomaritidine, 188f photochromism by diarylethenes, 176f Photooxygenation of (-)-β-citronellol, 191f synthesis of aminonaphthalene derivative, 181, 182f synthesis of duocarmycin, 181f synthesis of efaproxiral, batch/flow methodology, 180f synthesis of grossamide, 187f synthesis of 6-hydroxybuspirone, 184f synthesis of radiolabel 2-[18F]fluorodeoxyglucose (2-[¹⁸F]-FDG), 185f synthesis of symmetrical/unsymmetrical diarylethenes, 177f Kolbe-Schmitt reaction, 112 Lab-on-a-chip, 199 Langmuir-Hinshelwood mechanism, 86 Laplace pressure ($\Delta P_{Laplace}$), 20, 20f, 24, 32, 33 (MAUFs)

Laser-Raman scattering spectroscopy, 65 MAUFs. See Multi-attribute utility functions (MAUFs) Metal-catalyzed reactions, 145–148 continuous flow Heck–Mizoriki reaction, 146t continuous flow Suzuki–Miyaura reaction, 145t kinetic resolution of rac-4-hdroxy-1butene oxide, 146, 146f Suzuki-Miyaura coupling reactions, 147t Metal-organic framework (MOF), 87 MHCDs. See Micro hollow cathode discharges (MHCDs) Michael addition reaction, 123, 126, 126f Microcavity discharges, 42, 45, 45f

Microchemical (integrated) systems, design/ construction microchemical processes, example of, 6-14, 9t-10t multiphase microflow network, 5-6, 5f Microchemical processes, example of, 9t-10t Co wet analysis. See Micro cobalt wet analysis microimmunoassay clinical diagnosis, application/ limitation, 11, 12 design of, 12f heterogeneous immunoassay, 11 micro-ELISA system, 12, 13f molecular transport in microspace, 6-7 urine analysis conventional procedures, 13, 14f GC-MS technique, 13 microsystems for, 14f system design, MUOs/CFCP approach, Microchip electrophoresis, 5 Micro cobalt wet analysis CAD, application, 11 conventional procedures, 7 diffusion time dependence on diffusion length, 7f extraction/purification reactions, 8 system design, CFCP approach, 8f Microcountercurrent flow patterns, 27-31, 29f, 30f MicroELISA system, 3, 12, 13f Microfluidic droplet reactors, 206 Microfluidic fuel cell, 68 colaminar configuration, advantages, 68-69 example, 69f laminar flow characteristic, 68 Microfluidic reactors for nanomaterial synthesis automated microreactors application in nanotoxicology asbestos fibers, types, 225, 226f libraries of RMs, study, 227 "scale-out" process, benefits, 228 toxicity, influencing factors, 227 automated production of nanoparticles. See Automated microreactors

nanoparticle formation. See Formation of nanoparticles process control, 222--224 production of CdSe nanoparticles. See CdSe nanoparticles, production of synthesis of nanoparticles, microfluidic routes, 197-208. See also Formation of nanoparticles Micro hollow cathode discharges (MHCDs), 44-45, 44f Microplasma, 42 Microplasma reactors applications, 48-67 atmospheric pressure microplasmas, 41 - 48chemical synthesis in ammonia/CO2 decomposition, use of MHCD, 57-58 fabricated plastic microreactors, study (Anderson), 61 hydroxylation of benzene and toluene by DBD, 58-59, 58f oxidative conversion of C1-C3 alkanes by DBD, 59-60, 59f partial oxidation of methane, microreactor setup, 56-57, 57f Microreaction technology (MRT), 40, 104 Microreactors with electrical fields chemistry and electricity electrochemistry, 38 **MRT**, 40 plasma chemistry, 38. See also Plasma chemistry/technology electrochemical microreactors, 67-72 electrokinetic control of chemical reactions electrophoresis and electroosmosis, 72-77 electrowetting-on-dielectric, 81-82 positioning/trapping of particles/ molecules, 77-81 special effects, 82-85 electronic control of reactions at surfaces adsorption-desorption. See Adsorption-desorption by electrical fields control of activity of adsorbed molecules. See Adsorbed molecules, control of activity

Microreactors with electrical fields (Continued) microplasma reactors applications. See Applications of microplasma reactors atmospheric pressure microplasmas. See Atmospheric pressure microplasmas Microscopic quasielastic laser scattering method, 31 Microsegmented flows, 6 Micro-SMB separators, 71 Microunit operations (MUOs), 1-33 Microwave-assisted reactions bromination reactions, 115, 115f halide displacement reaction, 115, 115f Suzuki-Miyaura reaction, 114, 114f model for optimization of microwaveassisted reactions, 116t Wittig-Horner olefination, 115 Microwave irradiation, 111, 114 MOF. See Metal-organic framework (MOF) Molecular Dynamics or Monte Carlo simulations, 91 MRT. See Microreaction technology (MRT) MRT, high-throughput organic synthesis by advantages over batch vessels, 104-105 catalyst incorporation into microreactors acid-catalyzed microreactions, 140-144 base-promoted microreactions, 136-139 biocatalysis, 152-158 metal-catalyzed reactions, 145-148 multiple catalyst systems, 148-152 enhanced reaction control Domino reactions in a soda-lime microreactor, 105, 105f synthesis of 1,2-azoles by EOF, 105-106, 106t synthesis of chromenones, 106-107, 107f, 108t industrial applications. See Industrial applications of MRT photochemical reactions, 164-174 solid-supported reagents in noncatalytic flow processes heterogeneous photochemistry, 170-173 homogeneous photochemistry, 166-169

thermal control, 111-120 toxic/hazardous reagents, use of. See also Toxic/hazardous reagents in MRT continuous flow hydrosilylations using tris(trimethylsilyl)silane, 121t exothermic reactions, 135 fluorinations, 122-127 nitrations, 132-135 trimethylaluminum, 127 tris(trimethylsilyl)silane-mediated deoxygenation/dehalogenation reactions, 120-121 use of butyllithium in microreactors, 127-132 Multi-attribute utility functions (MAUFs), 220 Multiphase microflow(s) methods of stabilization, 25-32 physical properties. See Physical properties of multiphase microflows wettability-based microvalve, 32-33 Multiphase microflow network, 5-6, 5f electroosmotic flow, 5-6 microsegmented flows, 6 pressure-driven flow, 6 Multiple catalyst systems multistep synthesis of an α,β unsaturated compound, 149f polymer-assisted derivatization of steroid, 149f single pressure-driven flow reactor, use of solid-supported reagents, 150f synthesis of 2-(benzyloxy) tetrahydropyran, 151t Multiwalled carbon nanotubes (MWCNTs), 51 MUOs. See Microunit operations (MUOs) MUOs and CFCP integrated microchemical systems, design/construction microchemical processes, example of, 6 - 14multiphase microflow network, 5-6 microchemical chip/electronic system, comparison, 3f microtechnology, directions, 3-4 multiphase microflows fundamental physical properties, 14-25 methods of stabilization, 25-32 wettability-based microvalve, 32-33 MWCNTs. *See* Multiwalled carbon nanotubes (MWCNTs)

Nanostructure synthesis in microplasma reactors CNF growth, 51 microplasma in a capillary and in Pyrex chip, 52, 53f microreactor/catalyst coating/ microplasma treatment, 51, 52f synthesis of Fe/Ni catalyst particles (Chiang & Sankaran), 49 synthesis of MoO2 nanoparticles with UHF, 50-51, 50f synthesis of photoluminescent silicon nanocrystals by VHF, 49, 50f synthesis of silicon nanoparticles (Sankaran), 48, 49f UHF technique in MWCNTs, 51 Nanotechnology, 40 Nanowires, applications, 47 Nelder-Mead simplex procedure, 216 Nitrite conversion to oxime, 189, 189f Noise-free optimization, technique standard simplex method, 215, 215f, 216f "adaptive simplex" approach, 215, 217f "reflective-simplex" approach, advantages, 215, 216f statistical simplex approach, 218, 219f simultaneous optimization of peak emission wavelength and intensity, 220, 221f "Numbering up" principle, 54 Oligosaccharides, continuous flow synthesis, 119-120, 119f Oxomaritidine, flow-assisted synthesis, 188f PABA. See P-aminobenzoic acid (PABA)

PABA. See P-aminobenzoic acid (PABA) p-Aminobenzoic acid (PABA), 91 Paschen curve, 45, 46f PASSflow reactors, 148 PDMS microreactor, reactions conducted in, 154f–155f PEEK[™] tube, 12 Photochromism by diarylethenes, 176f

Photolithography, 26-27 Photooxygenation of (-)-β-citronellol, 191f Physical properties of multiphase microflows, 14-25 air-liquid microflows phase separation conditions, 24, 25f interfacial tension between air-solvent/ aqueous-organic interfaces at 20°C, 23t liquid-liquid microflows, 15f phase separation conditions, 23, 24f of multiphase microflows Laplace pressure ($\Delta P_{Laplace}$), 20, 21 liquid-liquid interface curves, 20f parallel multiphase microflows, equation, 21 pressure difference (ΔP_{Flow}), 20 two-phase microflows, 16-19, 17f viscosity of solvents at 20°C, 22t Plasma chemistry/technology electrokinetic transport of cahrges, forms DEP, 39 electroosmosis, 39 electrophoresis, 39 **EWOD. 39** industrial/commercial, examples atmospheric pressure plasmas, examples, 39 low-pressure discharge, examples, 38-39 Plasma-enhanced chemical vapor deposition (CVD), 38-39 Plasma state (fourth state of matter), 41 Point electrodes, 63, 66 Positioning/trapping of particles/molecules, 77 - 81Pressure-driven flow, 6, 74, 79, 81, 114, 150f, 164, 175 Pristane, continuous flow synthesis, 184-185, 185f Protein adsorption Derjaguin-Landau-Verwey-Overbeek theory, 92 orientation, experimental study atomic force microscopy, 92 SIMS, 92 orientation, theoretical study continuum models, 91-92 molecular models, 91 reversible and nonspecific, 89-90

Protein microarrays, 90 Pulsed electric fields, 84 QDQW. See Quantum-dot quantum-well (QDQW) Quantum-dot quantum-well (QDQW), 203-204 Radiolabel 2-[¹⁸F]-fluorodeoxyglucose (2-[¹⁸F]-FDG), synthesis of, 185f Reference materials (RMs), 227 Reynolds (Re) number, 15 Rimonabant, continuous flow synthesis, 180f RMs. See Reference materials (RMs) SAM. See Self-assembled monolayer (SAM) SAUFs. See Single attribute utility functions (SAUFs) "Scale-out" process, 228 Self-assembled monolayer (SAM), 26, 91, 93 Serpentine, 225, 226f Simplex method, 215, 216f. See also Noise-free optimization, technique Simulated moving bed (SMB), 70, 75 Single attribute utility functions (SAUFs), 220 SMB. See Simulated moving bed (SMB) Sonogashira C-C coupling reactions, 113 superheated water as reaction solvent, model reaction, 113f Spindt type field emitter, 47, 47f Spiro lactone derivative, continuous flow synthesis, 174f, 175t Stabilization methods, multiphase microflows chemical surface modification, 25. See also Chemical surface modification methods extraction processes microscopic quasielastic laser scattering method, 31 microcountercurrent flow patterns, 27, 29f liquid-liquid flows, 29, 30f plug flow to two-phase microflows, conversion, 27, 29f, 31-32 shape of the liquid-liquid interface in a microchannel, 25, 26f structure alteration, use of pillar structure, 25 Supercooled microflows, 118-119, 118f "Supersaturation" concentration, 197

Suzuki-Miyaura reaction, 114, 114f, 116, 145, 147 Synthesis of aminonaphthalene derivative, 132, 132f Synthesis of diarylethenes (symmetrical/ unsymmetrical), 177f Synthesis of oligosaccharides, continuous flow, 119-120, 119f Thermal control by MRT increased reaction temperature and pressure copper-free Sonogashira C-C coupling reactions, 113 dehydration of β-hydroxyketones, 112, 112f hydrolysis free O-acylation of alcohols, 114, 114f Kolbe-Schmitt synthesis of 2,4-dihydrobenzoic acid from resorcinol, 112, 112f microwave irradiation, alternative heat source. See Microwave-assisted reactions synthesis of α -aminophosphonates, 111, 111f reduced reaction temperatures alkylation of N-acyl oxazolidinone, 117, 117f continuous flow synthesis of oligosaccharides, 119-120, 119f decomposition of enolate, batch conditions, 117-118, 118f supercooled microflows application, scheme, 118, 118f Thermal lens microscope (TLM), 6f, 8.12 TLM. See Thermal lens microscope (TLM) TMSCN. See Trimethylsilyl cyanide (TMSCN) Toxic/hazardous reagents in MRT continuous flow hydrosilylations using tris(trimethylsilyl)silane, 121t exothermic reactions Paal-Knorr synthesis, 135 fluorinations of β-diketoester using elemental fluorine, 122, 122f

in small organic molecules (Miyake and Kitazume), 123, 126f substrates fluorinated by PTFE reactor (Gustafsson), 123, 124t trifluoromethylation of carbonyl compounds, 123, 125t nitrations of aromatics, 132-133 autocatalytic nitration of phenol, 133, 133f of salicylic acid, reaction products, 133-134, 134f selective nitration under flow by DSM, 134, 134f trimethylaluminum, 127, 128t tris(trimethylsilyl)silane-mediated deoxygenation/dehalogenation reactions, 120-121 use of butyllithium in microreactors anionic polymerizations under continuous flow, molecular weight effects, 131t benzophenone reactions in two-stage microreactor, 129 deprotonation of styrene oxide, reaction products, 131t monomer/initiator ratio, linear relation, 132 one-step coupling of fenchone/2bromopyridine. See Fenchone/2bromopyridine, one-step coupling

organometallics addition to benzophenone, 128f synthesis of aminonaphthalene derivative, 132, 132f Trifluoromethylation of carbonyl compounds, 123, 125t Trimethylaluminum, 127, 128t Trimethylsilyl cyanide (TMSCN), 143 Two-phase microflows, 16–19, 17f velocity profiles calculations, 18–19, 19f

UHF. See Ultrahigh frequency (UHF) Ultrahigh frequency (UHF), 50 Utility function, 212 UV photopatterning method, 27, 28f

"Viscous fingering," 74 VOCs. See Volatile organic compounds (VOCs) Volatile organic compounds (VOCs), 53

Wettability-based microvalve, 32-33, 32f Wittig-Horner olefination, 115, 182

Young-Laplace equation, 21 Y-shaped microfluidic device, design, 201, 201f residence time calculation, 201

Zeta potential, 73, 227, 228

Ref.660.2 ADV V.39

Note: The letters 'f' and 't' following locators refer to figures and tables respectively.

"Active" or "end-functionalized" chains, 144 Applications of mesoscale field-based models interaction of two grafted monolayers by attractive chains creation of stable dispersion, aim, 155 stable vs. unstable dispersion of tethered chains, 156f interaction of two grafted monolayers by end-functionalized chains analysis of density profiles at different gallery heights, 158-159, 160f calculated free energy profiles, SCFT approaches, 157-158, 157f calculated nanocomposite phase diagram, 160f Flory-Huggins interaction parameters used, 156t practical implications of the model, 161 predictions of the "compressible model." 161 interaction of two grafted monolayers with different segment sizes, 154, 155f interaction of two grafted monolayers with equal segment sizes density profiles of grafted/free polymers at separations, 148, 149f interpenetration of grafted monolayers/free polymer, 148 SCFT/iSAFT calculations, comparison, 148-154, 150f-153f of micro- and nanostructured materials, 132-133

structure of grafted polymer monolayers in a polymer melt, 147–148 comparison of density profiles, cases, 147f

Bioengineering, 76 Branched polymers gelation, 174–175 calculation of cyclic rank of polymer network (Flory theory), 175 gel point, 175 mathematical modeling of branched polymerization, objectives, 175 stochastic branching process, 173–174 Galton–Watson process, 174 Gordonian polymers, algorithm for, 174 tree/molecular forest, molecular graph representation, 174

Canonical-ensemble statistical mechanics, 88 CG-MC. See Coarse-grained Monte Carlo (CG-MC) CG-MD. See Coarse-grained molecular dynamics (CG-MD) Chapman-Enskog method, 122 Chemical correlators, 172-173 Chemical equilibrium, 90 Chemical modification of polymers PAR outlined theory for good/poor solvent, 187-188 PARs, example esterification of polymethacrylic acid, 186 neighboring-group (NG) model, 187 saponification of polyvinyl acetate, 186 Classical equilibrium thermodynamics, 2, 6, 8, 78-79, 81, 88, 106, 116-117 Clausius inequality, 4 Coal burning, interrelated processes burning of coke, 63-64 burning of volatiles, 63 coal pyrolysis, 63 Coal pyrolysis, 63 Coarse-grained molecular dynamics (CG-MD), 134 Coarse-grained Monte Carlo (CG-MC), 134 "Coarse-graining" process, 110 Coke burning, 63-64 Complex fluids, 76, 95, 110-111, 127 Contact geometry, 76-78, 80, 120 Continuous stirred tank reactor (CSTR), 190 Conventional free-radical copolymerization copolymerization of some monomers, anomalies in, 185-186 mathematical modeling, considerations, 186 quantitative theory of copolymerization short-range effects, types of kinetic models, 185 Convex programming (CP), 19 CSTR. See Continuous stirred tank reactor (CSTR) Denbigh, 190-191 Density functional theory (DFT), 134 DFT. See Density functional theory (DFT), 134 Dissipative macroscopic systems, equilibrium thermodynamic modeling of analysis of equilibrium models (Euler and Lagrange), 3 MEIS geometrical interpretations, 33-38 of spatially inhomogeneous systems, 26 - 28

with variable flows, 20-26

formalization, 29–33 MEIS application, examples of

with variable parameters, 17-20

formation of nitrogen oxides during

variants of kinetic constraints

coal combustion. 54-64

isomerization, 50-54

thermodynamics areas of computational efficiency, 46 - 50areas of effective applications, 39-46 "Model Engineering" (Gorban), 5 reversible and irreversible processes (Galileo), 3-4 substantiation for irreversible processes equilibrium and reversibility, interpretations, 8-11 equilibrium approximations, 16-17 experience of classics, 5-8 nonequilibrium thermodynamics, equilibrium interpretations of, 12-16 thermodynamics, emergence of principle of entropy (second law of thermodynamics), 3 thermodynamics of nonconservative systems, problems of analysis and development of MEISs, 70 analysis of computational problems in MEIS application, 70-71 reduction of models of irreversible motion to models of rest, 69-70 solution of specific theoretical/applied problems on MEIS, 71 Dissipative particle dynamics (DPD), 134 Distribution of the residence time (DRT), 191, 197 DPD. See Dissipative particle dynamics (DPD) DRT. See Distribution of the residence time (DRT) Equations of motion, 6 Equilibrium models, analysis of (Euler and Lagrange), 3 Equilibrium states, 91 Euler-Lagrange equations, 137 Extended Flory principle, 176-177, 184 Fenimore mechanism, 55-56

stationary flow distribution in

hydraulic circuits, 64-66

MEIS vs. models of nonequilibrium

Fenimore mechanism, 55–56
"Field-based" mesoscale theories. See Density functional theory (DFT) Flory-Huggins interaction parameters, 156t Flory principle, 176, 180, 184 Fluid mechanics, 105–113, 117–118, 122–127 "Free" or "matrix" homopolymer chains, 144 Fuel nitrogen oxides, formation of, 54–55

Galileo, 3 Galton-Watson branching process, 174 Gel, 175 Gelation, 174-175 Gel point, 175, 183 Gibbs paradox, 77 Gibbs phase rule, 16, 19, 47, 67 Gordonian polymers, 174-175, 178, 180, 183 Grafted polymer monolayers interaction by attractive chains creation of stable dispersion, aim, 155 stable vs. unstable dispersion of tethered chains, 156f interaction by end-functionalized chains analysis of density profiles at different gallery heights, 158-159, 160f calculated free energy profiles, SCFT approaches, 157-158, 157f calculated nanocomposite phase diagram, 160f Flory-Huggins interaction parameters used, 156t practical implications of the model, 161 predictions of the "compressible model," 161 interaction of, with different segment sizes, 154, 155f interaction of, with equal segment sizes density profiles of grafted/free polymers at separations, 148, 149f interpenetration of grafted monolayers/free polymer, 148 SCFT/iSAFT calculations, comparison, 148-154, 150f-153f structure in a polymer melt, 147-148 comparison of density profiles, cases, 147f

Henry law, 16 H-theorem, 3, 6 Hydraulic circuit theory, 24 Hydrodynamic fields, 106 Hydrodynamic stirring effects on properties of polymers effect on composition inhomogeneity, 195-196 general considerations advantages of continuous commercial processes over batch processes, 190 control of inhomogeneity of polymer, factors, 190 conventional radical polymerization systems, 191 degree of hydrodynamic stirring in PFR/CSTR, 190 living anionic polymerization systems, 191 statistical characteristics of a polymer, hierarchy, 189 microsegregation, 197 polycondensation, 194-195 polymer-analogous reactions, 196-197 radical polymerization, 191-194

Ideal kinetic model, 175-176 Irreversible processes, equilibrium thermodynamic modeling of equilibrium and reversibility, interpretations, 8-11 Boltzmann trajectories of motion, 9 dynamics of a system with periodic agitation (Gorban), 10, 10f equilibrium approximations, 11 equilibrium, main feature in mechanics, 8-9 "far from equilibrium," meaning (Gorban), 11 equilibrium approximations, 16-17 "damnation of dimension," 17 experience of classics, 5-8 classical equilibrium thermodynamics, computational tool used, 8 equilibrium and reversibility, analysis of interrelations, 6 equilibrium trajectories study and mathematical relations (Gibbs), 6-7 law of Fick, 8 partial equilibria notion, irreversible process of light diffusion, 8

Irreversible processes, equilibrium thermodynamic modeling of (Continued) principle of entropy increase (Boltzmann), 6 theory of electric circuits (Kirchhoff), 7 nonequilibrium thermodynamics, equilibrium interpretations of, 12-16 equilibrium interpretation of Prigogine theorem, situations (entropy equations), 12-14 Onsager reciprocal relations, 14-16 ISAFT model classical DFT, tool application in modeling interfacial properties of LJ fluid, 135-136 Helmholtz free energy as function of density distribution, basis, 136 prediction of microscopic structure/ thermodynamics/phase behavior, 135 extension to grafted polymer chains, 140-141 homogeneous systems PRISM, application, 136 Wertheim's TPT1, development of SAFT equation, 136 modeling of polyatomic molecules application in heterogeneous polymer systems, features, 140 density profile, expression, 139 ideal gas free energy functional, 138 linear polymer chain formation of msegments from m associating spheres, 137-140, 138f open system in canonical ensemble, free energy computation, 137-140 quantum DFT, 135 Isolated systems, study of (Gorban), 10, 10f Kinetic block of model, thermodynamic approaches constraint on process rate determined only by one reaction, 31-32 thermodynamic analysis of kinetic equations constraints used, 30-31 unity of thermodynamics and kinetics

constraints used, 29-30

Kinetic models of macromolecular reactions ideal kinetic model Flory principle, assumptions, 176 process of radical polymerization, 175-176 models allowing for the deviations from ideality extended Flory principle, 176-177 polymer nature of reagents, long-range effects, 177 substitution effects, short-range effects, 176 "Kink" mechanism, 161 Kirchhoff theorem of minimum heat production, 23 "Labeling-erasing" procedure, 181, 184, 185 Lagrange equilibrium equation, 6 Law of Fick, 8 Least action principle (PLA), 7, 16 Le Chatelier-Brown principle, 16 Legendre transformation, 76, 78-81, 83-85, 89, 92 Lennard-Jones (LJ) fluid, 136 "Living" radical polymerization (LRP), 193-194 LJ fluid. See Lennard-Jones (LJ) fluid LRP. See "Living" radical polymerization (LRP) Mass action laws, 16, 77, 99, 101, 175 Maximum entropy principle, 76, 81 'Mechanics,' 8 Mechanisms of NO formation, 54-56 MEIS. See Model of extreme intermediate states (MEIS) MEIS application, examples of formation of nitrogen oxides during coal combustion advantages of MEIS-based modeling, 64 coal burning, interrelated processes (kinetic models), 63-64 formulation of inequality by kinetic equations, 59 fuel nitrogen oxides, formation of, 54-55 kinetic constraints formulations in slow/fast subsystem, 57

NO formation from dinitrogen oxide, 56 prompt nitrogen oxides, formation of (Fenimore mechanism), 55-56 rate of nitrogen oxide formation, equation, 58 theoretical/experimental NO emissions at coal combustion, calculations, 61-62. 62f thermal nitrogen oxides, formation of (Zeldovich mechanism), 55 isomerization, 50-54 computational methods/accuracy, 52-54 constraint used, 50-51 graphical interpretation of isomerization process, 51f interpretation of studied problem, advantage, 52 kinetic equations for isomerization process, curves of, 53f "physico-economic" self-organization problem, analysis, 52 study of multistage processes, difficulties, 53 stationary flow distribution in hydraulic circuits, 64-66 final equilibrium model, form, 65 isothermal flow of incompressible fluid in three-loop circuit, example, 64-66 Prigogine theorem, aaplication, 66 results of flow distribution calculation, 66t scheme of the hydraulic circuit, 65f MEISs isomerization, 50-54 MEIS vs. models of nonequilibrium thermodynamics areas of computational efficiency, 46-50 areas of effective applications, 39-46 Mesoscale approaches, 134 Mesoscale field-based models, applications in polymer melts applications interaction of two grafted monolayers in presence of attractive chains, 154-155 interaction of two grafted monolayers in presence of end-functionalized chains, 156-161

interaction of two grafted monolayers with different segment sizes, 154 interaction of two grafted monolayers with equal segment sizes, 148-154 of micro- and nanostructured materials, 132-133 structure of grafted polymer monolayers in a polymer melt, 147-148 modeling of polymeric systems mesoscale approaches, 134 problems, 133 short-range structure, role in applications, 133 theory extension of iSAFT model to grafted polymer chains, 140-141 iSAFT model, 135-140 self-consistent field theory, 141-146 Microcanonical-ensemble statistical mechanics, 88 Microsegregation, 197 "Model Engineering," 5, 29, 39, 40, 68, 70 Model of extreme intermediate states (MEIS), 2 geometrical interpretations, 33-38, 35f hexane isomerization reaction, analysis, 36f. 37 idea of tree in formalization of macroscopic kinetic constraints, 38 notion of thermodynamic tree (Gorban), 36-38, 36f polyhedron of material balance, 34, 36f use of tree notion in constructing algorithms, 38 of spatially inhomogeneous systems, 26 - 28equations, 26-28 graph of spatially inhomogeneous system, 27f indication of harmful substance distribution in vertical air column, 28 macroscopic kinetics constraints inclusion, difficulties, 28 material balances in model, 28 parametric and flow MEIS features, 28 with variable flows, 20-26 construction of flow models of hydraulic systems, 24-26

Model of extreme intermediate states (MEIS) (Continued) "equilibrium" derivation, hydraulic circuit theory, 24 flow modifications, groups, 20 interpretation of flows as coordinates of states, 20 nonstationary flow distribution, equations, 23-24 stationary flow distribution in closed circuit, equations, 20-22 thermodynamic model of passive circuit, 22-23 with variable parameters, 17-20 convex programming (CP), 19 list of stages in model, need for indication, 19 model equations, assumptions, 18-19 variants of kinetic constraints formalization, 29-33 Boltzmann assumption, basis, 29 kinetic block of model, thermodynamic approaches, 29-32 MEIS modifications, difficulties, 32-33 "Model Engineering," 29 optimal description of constraints on macroscopic kinetics, issues, 33 Monads, 184 Multiscale equilibrium thermodynamics classical equilibrium thermodynamics, 78-79 mesoscopic equilibrium thermodynamics contact geometry, applications, 80-81 example: equilibrium kinetic theory (ideal gas), 81-84 example: equilibrium kinetic theory (van der Waals gas), 84-86 example: Gibbs equilibrium statistical mechanics, 86-89 example: multicomponent isothermal systems, 89-91 example: multicomponent nonisothermal systems, 91 fundamental thermodynamic relation, 79-80 Gibbs and Gibbs-Legendre manifolds, 81, 82f Multiscale nonequilibrium thermodynamics

combination of scales example: direct molecular simulations, 111-116 single scale realizations example: a simple illustration, 96-98 example: chemically reacting isothermal systems, 98-101 example: complex fluids, 110-111 example: fluid mechanics, 105-109 example: kinetic theory of chemically reacting systems, 101-105 example: particle dynamics, 109-110 Multiscale thermodynamics in chemical engineering Gibbs formulation of classical thermodynamics, 76 macroscopic/microstructure behavior of multicomponent systems, 76-77 multiscale equilibrium thermodynamics classical equilibrium thermodynamics, 78-79 mesoscopic equilibrium thermodynamics, 79-91 multiscale nonequilibrium thermodynamics combination of scales, 111-116 single scale realizations, 95-111 multiscale nonequilibrium thermodynamics of driven systems example: a simple illustration, 120-122 example: Chapman-Enskog reduction of kinetic theory to fluid mechanics, 122-127

Nano-engineering, 76 Neighboring-group (NG) model, 187 Nonconservative systems, 6, 9, 66, 69–71 Nonequilibrium thermodynamics, 4 Nonideal kinetic models, 180, 183

Opalescence phenomenon, 8

PARs. See Polymer-analogous reactions (PARs)

"Particle-based" mesoscale simulations. See Dissipative particle dynamics (DPD)

Paul Flory, 167, 178

PFR. See Plug flow reactor (PFR) PLA. See Least action principle (PLA) Plug flow reactor (PFR), 190 Polycondensation, 182-184, 194-195 choice of ideal kinetic model, 182-183 cross-linking of reactive oligomers, 182-183 extension of "substitution effect." 184 Gordonian polymers (branching process) "labeling-erasing" procedure, 183--184 monads, kinetically independent elements, 184 nonideal kinetic models, 183 statistical description of sol/gel molecules, 183 Polymer adsorption, 132 Polymer-analogous reactions (PARs), 186, 196-197 Polymer-clay nanocomposites, 134 dispersion in clay platelets, stabilization of, 135 equilibrium morphology of, 135 synthesis of, 134-135 Polymer properties, hydrodynamic stirring effects on effect on composition inhomogeneity, 195-196 general considerations advantages of continuous commercial processes over batch processes, 190 control of inhomogeneity of polymer, factors, 190 conventional radical polymerization systems, 191 degree of hydrodynamic stirring in PFR/CSTR, 190 living anionic polymerization systems, 191 statistical characteristics of a polymer, hierarchy, 189 🕚 microsegregation, 197 polycondensation, 194-195 polymer-analogous reactions, 196-197 radical polymerization, 191-194 Polymer reference interaction site model (PRISM), 136 Polymers, chemical modification of

PAR outlined theory for good/poor solvent, 187-188 PARs, example esterification of polymethacrylic acid, 186 neighboring-group (NG) model, 187 saponification of polyvinyl acetate, 186 Polymers, kinetic modeling of choice of model, considerations, 166-167 chemical modification of polymers, 167 polydispersity of products for synthesis, 167 description of polymers, peculiarities chemical correlators, 172-173 microstructure parameters, 171-172 quantitative description of macromolecules, problems, 168-169 statistical approach, 169-171 general theoretical results chemical modification of polymers, 186-188 conventional free-radical copolymerization, 184-186 polycondensation, 182-184 hydrodynamic stirring effects on properties of polymers effect of stirring on composition inhomogeneity, 195-196 microsegregation, 197 polycondensation, 194-195 polymer-analogous reactions, 196-197 radical polymerization, 191-194 kinetic models of macromolecular reactions ideal kinetic model, 175-176 models allowing for the deviations from ideality, 176-177 methods of calculations extension of statistical and kinetic methods, 180-182 kinetic method, 179-180 statistical method, 178-179 specificity of branched polymers gelation, 174-175 stochastic branching process, 173-174 Polymers, peculiar features in chemical correlators, 172-173 microstructure parameters, 171-172 statistical approach

Polymers, peculiar features in (Continued) isomerisms, types, 171 Markovian copolymers, features, 170 mathematical modeling for non-Markovian copolymers, 170 microstructure of copolymer molecules, characteristics of second group, 171 SCD function, characteristics of first group, 170 Principle of entropy, 3, 6 Principle of the least energy dissipation (Rayleigh), 7 Principles of statistical chemistry applied to kinetic modeling of polymers choice of model, considerations, 166-167 chemical modification of polymers, 167 polydispersity of products for synthesis, 167 description of polymers, peculiarities chemical correlators, 172-173 microstructure parameters, 171-172 quantitative description of macromolecules, problems, 168-169 statistical approach, 169-171 general theoretical results chemical modification of polymers, 186-188 conventional free-radical copolymerization, 184-186 polycondensation, 182-184 hydrodynamic stirring effects on properties of polymers effect of stirring on composition inhomogeneity, 195-196 microsegregation, 197 polycondensation, 194-195 polymer-analogous reactions, 196-197 radical polymerization, 191-194 kinetic models of macromolecular reactions ideal kinetic model, 175-176 models, allowing for the deviation from ideality, 176 methods of calculations extension of statistical and kinetic methods, 180-182 kinetic method, 179-180 statistical method, 178-179

specificity of branched polymers gelation, 174–175 stochastic branching process, 173–174 PRISM. *See* Polymer reference interaction site model (PRISM) Prompt nitrogen oxides, formation of, 55–56

Quantum theory of radiation (Beiträge), 16 Quasiparticles/"ghost" particles, 116

Radiation thermodynamics, 7–8 Radical polymerization, 175–176, 191–194 The Raoult law, 16

SCD. See Size-composition distribution (SCD) SCFT. See Self-consistent field theory (SCFT) Self-consistent field theory (SCFT), 134, 141-146 applications, 141 de Gennes-Edwards description of polymer molecule, 141 exfoliated/intercalated/immiscible morphologies, theories, 142 lattice model, schematic depiction, 143f free/active/grafted chain polymers, evaluation of propogators, 144-145 free energy/density profile, expressions, 143-145 nanocomposite phase diagrams, generation, 142 Single scale realizations in multiscale nonequilibrium thermodynamics example: a simple illustration, 96-98 example: chemically reacting isothermal systems, 98-101 example: complex fluids, 110-111 example: fluid mechanics, 105-109 example: kinetic theory of chemically reacting systems, 101-105 exchange-of-identity collisions, 105 inelastic collisions, 105 multicomponent systems with binary chemical reactions, 105 spatially nonlocal collisions, 105

example: particle dynamics, 109–110 Size-composition distribution (SCD), 170 Spatially inhomogeneous systems, 17, 26–28, 67, 70, 71 Stoichiometric coefficients, 90 Synergetics, 4, 12, 39, 46, 66, 67, 69

Theory of dynamic systems, 4, 12, 39, 67, 69, 167 Theory of electric circuits (Kirchhoff), 7 Thermal nitrogen oxides, formation of, 55 Thermodynamic Lyapunov functions, 3

٠

Thermodynamic perturbation theory (TPT1), 136 'Thermodynamics,' 3 TPT1. See Thermodynamic perturbation theory (TPT1) WAXS. See Wide-angle X-ray scattering (WAXS) Wertheim's thermodynamic perturbation theory, 136 Wide-angle X-ray scattering (WAXS), 142

Zeldovich mechanism, 55

Ref.660.2 ADV V.40



AB diblock copolymers under curved confinement, MC simulation of CMSC structure. See Complex multilayered sector column structure between concentric curved surfaces. 190-192 cylindrical pores, 187-190 Helmholtz energies, 204-206 under flat confinements, 190, 191 Helmholtz energy of, 186-187 morphologies of, 186, 188 MC simulated, 188-190 vertical and parallel lamellar structure of, 191, 192 Absorber and regenerators, separation models for, 145 Aggregates, gas-solids interphase momentum transfer, 30-31 Air bearing of HDI, flow inside, 109-112 Alkanolamine solution, CO₂ capture by, 136-137 Ammonia plants, 143 Aspen Plus EO model for. See Aspen Plus EO ammonia plant Aspen Plus EO ammonia plant blocks in, 144 CO₂ capture system optimization cases, 147-148 parameter cases, 146–147 S/C ratio, 147 execution times for, 146 gas composition optimization, 144 issues related to model specification in, 145

makeup stream, 145 optimization cases, 147 overall cycle time of, 146 separation models for absorber and regenerators, 145 Aspen Plus EO model for ammonia plant. See Aspen Plus EO ammonia plant for MDEA/PZ/CO₂ capture unit, 143 Asymmetrical concentric-ring barrel structure, Helmholtz energy of, 196-198 Asymmetrical concentric square column structure, Helmholtz energy of, 208 Athermal entropy of mixing, 162-163 Athermal mixture chemical potentials of, 162 probabilities of 1-1 pairs of, 163 Atomistic clusters, mapping of, 88 Atomistic MD simulations, 93 Atomistic/molecular-level modeling, 76-81 and integration, 87-89

Binary ising lattice, coexistence curves of, 166
Binary polymer solutions coexistence curve of, 168–169 normalized internal energy of mixing for, 171
Block copolymer melts. *See also* AB diblock copolymers
Helmholtz energy of, 185 micro-phase separation with multidimensional confinements, 185–186 morphologies of effect of disperse index on, 186 factors controlling, 184, 185 variety of, 186 Boltzmann transport equation and SRS models, 91 Bonding mechanism between PFPEs and overcoat, 72 BTE. See Boltzmann transport equation Bubble columns physical explanation of regime transition in, 41–42 total energy dissipation and, 40 Bubble phenomenon in situ, 99–100

Carnahan-Starling equation for hard-sphere fluids, 158 Catalyst (particle), reaction mechanism over.3 CFB combustors components of, 46 EMMS-based multi-scale CFD simulation coal combustion, 51 hydrodynamics, 48-49 seesaw phenomenon, 50 solid fluxes, 49-50 scale-up and optimal design of, 47 CFB risers components of, 21 ETH riser, 22-23 IPE riser, 21 simulations of, 21 voidage profiles of, 21-22 CFD simulations, 47 Chain-like molecular systems, mixing process of, 160 Chemical engineering, multi-scale characteristics of, 3 Chemical reactors multi-scale characteristics of, 2-4 need for scale-up of, 4-5 "overall" reaction behavior of, 4 scales involved in, 3 Chemical supply chain, multiscale process modeling of, 122 Classical molecular simulation methods, 76 Classic chemical engineering models, 10

Close-packed lattice model, 157 Cluster accelerations, X-ray measurement of. 6–7 Clustering, 13 Cluster velocity series determination, 7 Coarse-grained, bead-spring model of PFPE lubricant films, 104-105 with flat surface assumption, 105-106 potential energy characteristics, 106 Coarse-graining methods meso-scale---continuum levels, 91-92 molecular—meso-scale levels, 89–90 quantum-atomistic/molecular levels, 87-89 Cobalt (Co)-based magnetic alloys, 69 CO₂ capture by aqueous alkanolamine solution, 136 - 137with aqueous MDEA/PZ solution aqueous phase reactions, 138 chemical species considered for, 138 mechanism of action, 137 thermophysical properties of, 139 with chemical absorbent, 142 process modeling absorber and stripper, 140 and ammonia plant, 143-148 Aspen Plus EO model for, 143–144 equilibrium-stage models for, 141 performance correlations, 143 rate-based multistage separation models for. 141-142 Coexistence curves of binary polymer solutions, 168-169 of branched polymer solutions, 169 of lattice random copolymers, 170 of tert-butyl acetate/PS and water/poly (ethylene glycol) systems, 174 Complex multilayered sector column structure under curved confinements, 206-207 Helmholtz energy of, 207-209 Computational fluid dynamics, 3 correlative. See correlative multi-scale CFD space resolution of, 10 Continuously stirred tank reactor (CSTR) model, 10 Correlative multi-scale CFD challenges associated with, 14-15

computation cost effectiveness of, 13 paradigms for, 12 for single-phase turbulent flows, 12 subparticle simulations using, 12–13 and variational, comparison between, 17 Curved surfaces, MC simulation of diblock copolymers confined in between concentric curved surfaces, 190–192 cylindrical pores, 187–190

DDFT based on equation of state (EOS-based DDFT) applications of, 156 Degrees of freedom (DOFs), 126 in optimization, 127 Dense "cluster" phase, 5 velocities with respect to, 6 Dense-phase momentum balance, 25 Density functional theory (DFT), 75 Diblock copolymers confined in curved surfaces, MC simulation of between concentric curved surfaces, 190-192 cylindrical pores, 187-190 confined in ring-like curved surfaces, SSL theory for, 192 Helmholtz energy of asymmetrical parallel lamellar, 196–198 Helmholtz energy of sector column, 198-199 Helmholtz energy of symmetrical parallel lamellar, 193-196 under flat and curved confinements. 190, 191 Helmholtz energy of, 186-187 morphologies of, 186, 188 phase separation of confined, 209-210 vertical and parallel lamellar structure of, 191, 192 Dilute "broth" phase, 5 velocities with respect to, 6 Dilute-phase momentum balance, 25 Direct methanol fuel cell, 64 fuel in, 65 vs. hydrogen fuel cells, 65 Direct numerical simulations computational demand of, 11

of gas-solid suspension, 11 limitation on scalability, 10-11 Disk overcoat and PFPEs, interaction between, 71-72 bonding mechanism between, 72 DDPA-S, DDPA-D, and ZTMD, 72 DMFC. See Direct methanol fuel cell Drag coefficient in CFB, 8-9 Dry surfaces nanotribology of, 67 Dual-Bubble-Size (DBS) model for gas-liquid two-phase flow in bubble columns calculation on structure parameters and total gas holdup, 41 CFD simulation, 42–43 components of, 40 regime transition in bubble columns, 41 - 42Dynamic structure, 5

Electrostatic effects, modeling of, 76-77 Embedded solution strategy, 131-132 EMMS-based multi-scale CFD flow regime diagrams of CFB, 32 industrial applications CFB boiler, 46-51 fluid catalytic cracking, 43–46 EMMS model. See Energy-minimization multi-scale model Endbead density profiles for PFPEs, 106-107 Energy-minimization multi-scale model application of choking point prediction in fastfluidization, 26 mass/heat transfer and reactions. 35-40 and CFD, coupling of two-step scheme for, 27-29 voidage profile and, 30 closure of, 26 formulation of, 25-26 meso-scale heterogeneity of, 24-25 Equation-oriented (EO) modeling, 121 embedded solution strategy, 131 EO model-based RTO applications, 134 and sequential modular modeling, 123

Equilibrium-based models, absorber and regenerators, 145 ETH CFB simulation, 31

FCC. See Fluid catalytic cracking FCC-air system, 27 flow regime diagrams for, 32-33 H_D for, 30 heterogeneity index for, 30 Fertilizer site complex major facilities of, 148-149 optimization model CO₂ compressor, 149-150 of site steam system, 150 urea reactor, 149 schematic representation of, 149 Flory-Huggins lattice theory, 158 Flow regime diagrams of CFB for air-FCC system and air-HGB system, 32-33 apparent and intrinsic, 33-34 dependency on riser height, 34 Fluid catalytic cracking, 43 Fluidized bed, factors affecting meso-scale clusters in, 15 Fluidized bed reactors multiphase flow in, 10-11 range of solids fraction, 5 single particle for, 4 Fluidized systems simulated, physical properties of, 18 Fluid-particle interactions, 4, 11 Fomblin Z derivatives, 71

Gas and solid phases, slip velocity between, 13 Gas-liquid systems in bubble columns, 40 EMMS modeling of, 40–43 Gas-solid suspensions direct numerical simulations of, 11 heterogeneous structures in, 13 Gas-solid systems DNS simulation of, 14 meso-scale effects of, 14 ''Global reaction'', 3

Hard disk drive commercialized lubricant for, 70, 71

components of, 67, 68 as data storage systems, 67 headdisk interface of components of, 68, 69 cross-sectional diagram of, 70 lubricant film, 70 multi-scale integration atomistic simulations for, 103 coarse-grained MD models for, 103-107 meso-scale/continuum level, 109-112 simple reactive sphere model for, 108-109 nanotribology in, 69 read/write head, 73 structure of, 69 Harmonic potential energy, 77 HDD. See Hard disk drive HDI. See Head disk interface Head disk interface components of, 68, 69 cross-sectional diagram of, 70 flow inside air bearing of Knudsen number flow regime, 109-110 slip velocity on wall, 110 lubricant film, 70 magnetic head in, 73-74 multi-scale modeling of, 101 Heat transfer, EMMS model application in, 38-39 Helmholtz energy model of mixing applications of, 156 expression for, 159-160 molecular parameters in, 156 for multicomponent Ising mixture, 163-166 for polymers based on close-packed lattice model, 159-162 Helmholtz energy of mixing of polymer systems, 167 for two-step mixing process, 172 Heterogeneity index, 6 Heterogeneous structures in gas-solid suspensions, 13 Hierarchical multi-scale model, 84 structure of atomistic/molecular level, 76-81 meso-scale/continuum level, 81-83 process-scale level, 83-84 quantum level, 75-76

Homopolymer solution, lattice density functional for equilibrium density distribution, 182 excess Helmholtz energy functional, 179–181 grand potential, 181 at solid–liquid interface, 182–184 Hydrogen PEFC components of, 63, 64 uses of, 63 working principle of, 63, 64

IBM 3370 head, 73 Industrial process models applications, 134-135 critical success factors for successful, 135 fidelity of, 130-131 maintenance of, 133-134 for monitoring equipment/process performance, 126 objectives, 124 offline and online usage, 132-133 for optimization, 127-128 parameter estimation with, 126 and process economics, 132 for reconciliation, 126-127 scope of, 130 for simulation studies, 125-126 variables, 124-125 Interphase forces and reactor behavior, 8 Intrinsic flow regime diagram for air-FCC system, 33 "Intrinsic reaction", 3-4 Ising mixture, 163 Helmholtz energy of mixing for, 165-166 internal energy of mixing of, 164

Knudsen number of air bearing of HDI, 109 normalized velocity profiles at various values of, 110–111 streamlines of cavity flow at, 111–112

Lattice Boltzmann method, 83 kinetic models, 82 as multi-scale simulation tool, 81 for porous media flow simulation, 97 REV, 99 and SRS models, 91

Lattice cluster theory, 158-159 Lattice density functional theory for homopolymer solution equilibrium density distribution, 182 excess Helmholtz energy functional, 179-181 grand potential, 181 at solid-liquid interface, 182-184 for polymer adsorption, 177-178 for segment-density distributions, 183-184 Lattice fluid model, 157 EOS based on, 175 Lattice model. See also Ising mixture applications for phase equilibria calculations, 173 lattice fluid molecular thermodynamic model, 174 Flory-Huggins lattice theory, 158 grand potential for, 181 molecule arrangement in, 156-157 problems associated with, 158 LBM. See Lattice Boltzmann method LCT. See Lattice cluster theory LDFT. See Lattice density functional theory LDFT equation for equilibrium distribution, 181-182 near a planar solid surface, 182–183 Lennard-Jones potential, 76 Linear programming (LP) models, 121 Liquid film for CO₂ capture with chemical absorbent, 141–142 Liquid-liquid equilibria phase diagrams of ternary polymer solutions, 170-171 for [R_nmim][PF₆] + Butan-1-ol system, 175 Lubricant films characteristics of ideal, 70 first line of protection from mechanical damage, 70 PFPEs, 71 chemical structure of, 71 and disk overcoat, interaction between, 71-72 bonding mechanism between, 72 DDPA-S, DDPA-D, and ZTMD, 72

Macro-scale, 4 Magnetic head slider, 74 Mass transfer

in CFB, 8-9 EMMS model application in, 35-38 MC simulation. See Monte Carlo simulation MD. See Molecular dynamics MDEA. See n-Methyldiethanolamine MDEA-CO2-water system, CO2 partial pressures for, 139-140 MD simulation, atomistic, 87, 89 Meso-scale, 4 Mesoscale clusters and dispersed particles, exchange between, 8 Meso-scale/continuum-level modeling tool, 81-83 Meso-scale modeling, macro-scale influence into, 15 Meso-scale structures, 2 classic chemical engineering models for, 10of copolymer materials, 155 critical effect of, 8-9 drag coefficient and mass transfer for CFB due to, 8-9 in gas-solid suspensions, 13 particle behaviour in, 4 related to processes, 155 spatiotemporal features of dynamic characterizations, 6-8 time-averaged characterization, 5-6 TFM grid refining and, 23-24 two-phase description of, 5-6 n-Methyldiethanolamine, 145 CO₂ capture with, 137-138 molecular structure of, 137 Microkinetics-based reactor models, 135 Micro-phase structure formation mechanism for block copolymers, 184 Micro-scale, 4 MIP reactor, industrial flow regime diagram of, 46 simulation of, 45 solids volume fraction in laboratoryscale cold model of, 44 Mixing process of chain-like molecular systems, 160 Modified Reynolds equation, 109 Molecular dynamics, 78 and MC, 78 molecular motion in, 79-81 Molecular system, 75 Molecular thermodynamic model, 156

Monte Carlo simulation, 78 of CMSC structure, 206, 209 of diblock copolymers confined in curved surfaces between concentric curved surfaces, 190-192 cylindrical pores, 187-190 $N_{layer}vs. R_{ex}/L_0$ in, phase separation of diblock copolymer, 201-204, 209 and SSL theory, conflict between, 206 MRE. See Modified Reynolds equation Multiphase chemical reactor, 2-4 Multiphase flow in fluidized bed reactors, 10 - 11Multiphenomena in gas diffusion layer, 97-102 "Multi-scale CFD" applications periodic domain simulations, 16-21 scope of, 23-24 simulations of risers and validations, 21 - 23correlative challenges associated with, 14–15 computation cost effectiveness of, 13 paradigms for, 12 for single-phase turbulent flows, 12 subparticle simulations using, 12 - 13definition, 12 variational challenges to, 15-16 definition of, 15 scale separation condition in, 15 Multi-scale modeling approaches, candidates for evaluating HDD system, 66-74 PEFC, 63-66 at atomistic/molecular level, 76-81 bridging methodology, 85-87 of chemical supply chain, 122 components, 74-75 demand for research in, 113 at meso-scale/continuum level, 81-83 as multidisciplinary analysis paradigm, 60 at process-scale level, 83-84 publications on, 62 at quantum level, 75-76 schematic description of, 61

Multi-scale models, 122 coupling of bridging procedure for, 85–87 challenges associated with, 86 coarse-graining methods. *See* Coarse-graining methods need for developing, 61 publications on, 62 time and length scales in, 62 Multi-scale simulation, 61 Multi-scale structures, 2

Nafion[#], 65 Nanoanalysis, advances in, 60 Nanopore Helmholtz energy confined in, 187 layer transitions in, 204 Negative pressure heads, 73 Nonlinear nonequilibrium system, 16

Objective functions, 127 Ono-Kondo equation, 177 Optimization methods, 127–128

Parameter cases, 128-129 Particle-particle interaction, 11 PEFC. See Polymer electrolyte fuel cells PEFC-based power plant, process-level model of, 64 PEFC model device-level, 102 multiphenomena in gas diffusion layer, 97-102 polymer electrolyte membrane ab initio models of, 93 composition of, 92–93 water uptake variation in, 94–96 process-level, 102-103 water management strategies in, 65-66 PEM. See Polymer electrolyte membrane PEM materials functions, 65 Nafion[®], 65 PEM systems, water management issues in. 66 Periodic domain simulations, periodic 2D domains, 16 domain-size dependency of, 20 grid-size dependency of, 20-21

grid size estimation, 17 physical properties, 17-18 time-averaged dimensionless slip velocity grid resolution effects on, 18-19 periodic domain size effects on, 19, 21 two-phase flow, 18 PFPE lubricant films, coarse-grained, bead-spring model of, 104-105 PFPE molecule oligomeric, rigid units of, 89-90 PFPE Zdol molecule, molecular model of. 105 radius of gyration of, 108 PFPEs, functional and nonfunctional endbead density profiles for, 106-107 spreading profile of SRS models with, 107 PFPE systems, 71 and disk overcoat, interaction between, 71 - 72bonding mechanism between, 72 DDPA-S, DDPA-D, and ZTMD, 72 molecular conformation of, 108 Physical system, multi-scale/holistic interpretation of, 101 Piperazine, 137 Plug-flow model, 10 PNIPAm gels, swelling ratio of, 175 Polymer adsorption based on lattice or off-lattice model, 176 at interface, importance of, 176 lattice-based theories for, 177 DFT, 177 general formalism for, 178-179 LDFT, 177-182 at solid-liquid interface, 182-184 Polymer chains, residual Helmholtz energy of dissociation and association of, 166-167 Polymer electrolyte fuel cells component of, 63 design, 66 key issues in making paradigm shift in, 66 Polymer electrolyte membrane, 63 ab initio models of, 93 components of, 92 composition of, 92-93 water uptake variation in, 94–96 Polymer systems

based on lattice fluid model, equation of state for, 171-173 close-packed lattice model for, 159 comparisons with molecular simulation results coexistence curves, 168-170 critical temperature and critical volume fraction, 167-168 liquid-liquid phase equilibria, 170 - 171Helmholtz energy of, 178 Helmholtz energy of mixing of, 167 Polystyrene-b-polybutadiene (PS-b-PBD) diblock copolymers confined in nanopore comparison with MC simulation and SSL theory, 201-204 Helmholtz energy profiles of, 200-201 morphologies of, 199 Primary reformer feed steam to carbon (S/C) ratio, 147 Process economics, 132 Process-scale models, 83-84 PS/cyclohexane systems, spinodal curves and coexistence curves of, 174 PZ. See Piperazine

Quantum level models coupling of, 87–89 quantum level models, 75–76

Real-time optimization (RTO) applications, 134 Reconcile case, 129 Reconciliation models, 126-127 Reduced-order models approximation errors, 87 different forms of, 86-87 linking models at various scales using, 85-86 role of, 86 Representative elementary volume (REV) method, 97, 98 Reverse Monte Carlo (RMC) techniques, 88 Ring-like curved surfaces, 192 Helmholtz energy of asymmetrical parallel lamellar confined in, 196-198 Helmholtz energy of sector column confined in, 198-199

Helmholtz energy of symmetrical parallel lamellar confined in, 193-196 ROMs. See Reduced-order models Sector column structure Helmholtz energy of, 198-199 Semilean and lean solution columns, 147 Sequential modular (SM) modeling and equation-oriented (EO) modeling, 123 "Simulate" cases, 128 Slip velocity asymptotic, 19 grid resolution effects on, 18-19 periodic domain size effects on, 19 Solid particles, heterogeneity in, 6 SRS models, 89-90, 91 with spins, 108 spreading profile of PFPEs, 107-108 SSL theory. See Strong Segregation Limit theory Static structures, microscale difference of, 5 Strong Segregation Limit theory, 185 for diblock copolymers confined in ring-like curved surfaces, 193–199 Helmholtz energies predicted by, 205-206 N_{layer}vs. R_{ex}/L₀ in, 201-204 phase separation of confined diblock copolymer, 209-210 Subgrid structure modeling, 23 Subparticle simulations, 12-13 Symmetrical concentric-ring barrel structure Helmholtz energy of, 193-196 Symmetrical concentric square column structure, Helmholtz energy of, 207-208

Ternary Ising lattice internal energy of mixing for, 166 Ternary polymer solutions, liquid-liquid equilibria phase diagrams of, 170–171 TFM. See Two-fluid model Thermal 40 mers, total segment-density distributions of, 184 Tribology, 66–67 Turbulent flows, transfer of energy in, 15 Two-fluid model. See also Periodic domain simulations, periodic 2D domains applicability for for bubbling fluidized bed, 23 fine-grid and coarse-grid, 11 grid refining and meso-scale structures, 23–24 Two-step mixing process, 172 challenges to, 15–16 and correlative, comparison between, 17 definition of, 15 scale separation condition in, 15

Water uptake variation in PEM, 94-96

Vapor-liquid equilibria for propanol + [Me₃BuN][NTf₂] system, 175 Variational multi-scale CFD

Ztetraol multidentate, 72 ZTMD. See Ztetraol multidentate