SUBJECT INDEX

AB diblock copolymers

	maneup stream, 110
under curved confinement, MC	optimization cases, 147
simulation of	overall cycle time of, 146
CMSC structure. See Complex	separation models for absorber and
multilayered sector column	regenerators, 145
structure	Aspen Plus EO model
between concentric curved surfaces,	for ammonia plant. See Aspen Plus EO
190–192	ammonia plant
cylindrical pores, 187–190	for MDEA/PZ/CO ₂ capture unit, 143
Helmholtz energies, 204–206	Asymmetrical concentric-ring barrel
under flat confinements, 190, 191	structure, Helmholtz energy of,
Helmholtz energy of, 186-187	196–198
morphologies of, 186, 188	Asymmetrical concentric square column
MC simulated, 188–190	structure, Helmholtz energy of, 208
vertical and parallel lamellar structure	Athermal entropy of mixing, 162–163
of, 191, 192	Athermal mixture
Absorber and regenerators, separation	chemical potentials of, 162
models for, 145	probabilities of 1–1 pairs of, 163
Aggregates, gas-solids interphase	Atomistic clusters, mapping of, 88
momentum transfer, 30–31	Atomistic MD simulations, 93
Air bearing of HDI, flow inside, 109-112	Atomistic/molecular-level modeling,
Alkanolamine solution, CO ₂ capture by,	76–81
136–137	and integration, 87–89
Ammonia plants, 143	_
Aspen Plus EO model for. See Aspen	
Plus EO ammonia plant	Binary ising lattice, coexistence curves of,
Aspen Plus EO ammonia plant	166
blocks in, 144	Binary polymer solutions
CO ₂ capture system	coexistence curve of, 168-169
optimization cases, 147-148	normalized internal energy of mixing
parameter cases, 146–147	for, 171
S/C ratio, 147	Block copolymer melts. See also AB diblock
execution times for, 146	copolymers
gas composition optimization, 144	Helmholtz energy of, 185
issues related to model specification in,	micro-phase separation with multidi-
145	mensional confinements, 185-186

makeup stream, 145

morphologies of	Close-packed lattice model, 157
effect of disperse index on, 186	Cluster accelerations, X-ray measurement
factors controlling, 184, 185	of, 6–7
variety of, 186	Clustering, 13
Boltzmann transport equation	Cluster velocity series determination, 7
and SRS models, 91	Coarse-grained, bead-spring model of
Bonding mechanism between PFPEs and	PFPE lubricant films, 104–105
overcoat, 72	with flat surface assumption, 105-106
BTE. See Boltzmann transport equation	potential energy characteristics, 106
Bubble columns	Coarse-graining methods
physical explanation of regime	meso-scale—continuum levels, 91–92
transition in, 41–42	molecular—meso-scale levels, 89-90
total energy dissipation and, 40	quantum—atomistic/molecular levels,
Bubble phenomenon in situ, 99–100	87–89
r	Cobalt (Co)-based magnetic alloys, 69
	CO ₂ capture
Carnahan–Starling equation for	by aqueous alkanolamine solution,
hard-sphere fluids, 158	136–137
Catalyst (particle), reaction mechanism	with aqueous MDEA/PZ solution
over, 3	aqueous phase reactions, 138
CFB combustors	chemical species considered for, 138
components of, 46	mechanism of action, 137
EMMS-based multi-scale CFD	thermophysical properties of, 139
simulation	with chemical absorbent, 142
coal combustion, 51	process modeling
hydrodynamics, 48-49	absorber and stripper, 140
seesaw phenomenon, 50	and ammonia plant, 143–148
solid fluxes, 49–50	Aspen Plus EO model for, 143–144
scale-up and optimal design of, 47	equilibrium-stage models for, 141
CFB risers	performance correlations, 143
components of, 21	rate-based multistage separation
ETH riser, 22–23	models for, 141–142
IPE riser, 21	Coexistence curves
simulations of, 21	of binary polymer solutions, 168-169
voidage profiles of, 21–22	of branched polymer solutions, 169
CFD simulations, 47	of lattice random copolymers, 170
Chain-like molecular systems, mixing	of tert-butyl acetate/PS and water/pol
process of, 160	(ethylene glycol) systems, 174
Chemical engineering, multi-scale	Complex multilayered sector column
characteristics of, 3	structure
Chemical reactors	under curved confinements, 206-207
multi-scale characteristics of, 2-4	Helmholtz energy of, 207–209
need for scale-up of, 4–5	Computational fluid dynamics, 3
"overall" reaction behavior of, 4	correlative. See correlative multi-scale
scales involved in, 3	CFD
Chemical supply chain, multiscale process	space resolution of, 10
modeling of, 122	Continuously stirred tank reactor (CSTR)
Classical molecular simulation methods,	model, 10
76	Correlative multi-scale CFD
Classic chemical engineering models, 10	challenges associated with, 14–15
0	0

computation cost effectiveness of, 13 of gas-solid suspension, 11 paradigms for, 12 limitation on scalability, 10-11 for single-phase turbulent flows, 12 Disk overcoat and PFPEs, interaction subparticle simulations using, 12-13 between, 71-72 and variational, comparison bonding mechanism between, 72 DDPA-S, DDPA-D, and ZTMD, 72 between, 17 DMFC. See Direct methanol fuel cell Curved surfaces, MC simulation of diblock copolymers confined in Drag coefficient in CFB, 8-9 between concentric curved surfaces, Dry surfaces 190-192 nanotribology of, 67 cylindrical pores, 187-190 Dual-Bubble-Size (DBS) model for gas-liquid two-phase flow in bubble columns DDFT based on equation of state calculation on structure parameters and (EOS-based DDFT) total gas holdup, 41 applications of, 156 CFD simulation, 42-43 Degrees of freedom (DOFs), 126 components of, 40 in optimization, 127 regime transition in bubble columns, Dense "cluster" phase, 5 velocities with respect to, 6 Dynamic structure, 5 Dense-phase momentum balance, 25 Density functional theory (DFT), 75 Diblock copolymers Electrostatic effects, modeling of, confined in curved surfaces, MC 76 - 77simulation of Embedded solution strategy, 131-132 between concentric curved surfaces, EMMS-based multi-scale CFD 190-192 flow regime diagrams of CFB, 32 cylindrical pores, 187–190 industrial applications confined in ring-like curved surfaces, CFB boiler, 46-51 fluid catalytic cracking, 43-46 SSL theory for, 192 EMMS model. See Energy-minimization Helmholtz energy of asymmetrical parallel lamellar, 196-198 multi-scale model Helmholtz energy of sector column, Endbead density profiles for PFPEs, 198-199 106-107 Helmholtz energy of symmetrical Energy-minimization multi-scale model parallel lamellar, 193-196 application of under flat and curved confinements, choking point prediction in fast-190, 191 fluidization, 26 Helmholtz energy of, 186-187 mass/heat transfer and reactions, morphologies of, 186, 188 35 - 40phase separation of confined, and CFD, coupling of 209-210 two-step scheme for, 27-29 vertical and parallel lamellar structure voidage profile and, 30 of, 191, 192 closure of, 26 Dilute "broth" phase, 5 formulation of, 25-26 velocities with respect to, 6 meso-scale heterogeneity of, 24-25 Dilute-phase momentum balance, 25 Equation-oriented (EO) modeling, 121 Direct methanol fuel cell, 64 embedded solution strategy, 131 fuel in, 65 EO model-based RTO applications, vs. hydrogen fuel cells, 65 Direct numerical simulations and sequential modular modeling, computational demand of, 11

Equilibrium-based models, absorber and	components of, 67, 68
regenerators, 145	as data storage systems, 67
ETH CFB simulation, 31	headdisk interface of
	components of, 68, 69
	cross-sectional diagram of, 70
FCC. See Fluid catalytic cracking	lubricant film, 70
FCC-air system, 27	multi-scale integration
flow regime diagrams for, 32–33	atomistic simulations for, 103
H_D for, 30	coarse-grained MD models for,
heterogeneity index for, 30	103–107
Fertilizer site complex	meso-scale/continuum level, 109–112
major facilities of, 148–149	
	simple reactive sphere model for, 108–109
optimization model	
CO ₂ compressor, 149–150	nanotribology in, 69
of site steam system, 150	read/write head, 73
urea reactor, 149	structure of, 69
schematic representation of, 149	Harmonic potential energy, 77
Flory–Huggins lattice theory, 158	HDD. See Hard disk drive
Flow regime diagrams of CFB	HDI. See Head disk interface
for air–FCC system and air–HGB	Head disk interface
system, 32–33	components of, 68, 69
apparent and intrinsic, 33–34	cross-sectional diagram of, 70
dependency on riser height, 34	flow inside air bearing of
Fluid catalytic cracking, 43	Knudsen number flow regime,
Fluidized bed, factors affecting meso-scale	109–110
clusters in, 15	slip velocity on wall, 110
Fluidized bed reactors	lubricant film, 70
multiphase flow in, 10–11	magnetic head in, 73-74
range of solids fraction, 5	multi-scale modeling of, 101
single particle for, 4	Heat transfer, EMMS model application in
Fluidized systems simulated, physical	38–39
properties of, 18	Helmholtz energy model of mixing
Fluid–particle interactions, 4, 11	applications of, 156
Fomblin Z derivatives, 71	expression for, 159–160
	molecular parameters in, 156
	for multicomponent Ising mixture,
Gas and solid phases, slip velocity	163–166
between, 13	for polymers based on close-packed
Gas-liquid systems	lattice model, 159–162
in bubble columns, 40	Helmholtz energy of mixing
	of polymer systems, 167
EMMS modeling of, 40–43 Gas–solid suspensions	for two-step mixing process, 172
direct numerical simulations of, 11	Heterogeneity index, 6
heterogeneous structures in, 13	Heterogeneous structures in gas-solid
Gas-solid systems	suspensions, 13
DNS simulation of, 14	Hierarchical multi-scale model, 84
meso-scale effects of, 14	structure of
"Global reaction", 3	atomistic/molecular level, 76–81
	meso-scale/continuum level,
	81–83
Hard disk drive	process-scale level, 83–84
commercialized lubricant for, 70, 71	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	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
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	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
Interphase forces and reactor behavior, 8 Intrinsic flow regime diagram for air–FCC system, 33	Liquid film for CO ₂ capture with chemical absorbent, 141–142 Liquid–liquid equilibria
"Intrinsic reaction", 3–4	phase diagrams of ternary polymer
Ising mixture, 163 Helmholtz energy of mixing for, 165–166 internal energy of mixing of, 164	$\begin{array}{c} \text{solutions, } 170171 \\ \text{for } [R_n \text{mim}][PF_6] + \text{Butan-1-ol system,} \\ 175 \\ \text{Lubricant films} \end{array}$
Knudsen number of air bearing of HDI, 109 normalized velocity profiles at various values of, 110–111 streamlines of cavity flow at, 111–112	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
Lattice Boltzmann method, 83 kinetic models, 82 as multi-scale simulation tool, 81	DDPA-S, DDPA-D, and ZTMD, 72

for porous media flow simulation, 97

REV, 99

and SRS models, 91

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

in CFB, 8–9	Monte Carlo simulation, 78
EMMS model application in, 35–38	of CMSC structure, 206, 209
MC simulation. See Monte Carlo	of diblock copolymers confined in
simulation	curved surfaces
MD. See Molecular dynamics	between concentric curved surfaces,
MDEA. See n-Methyldiethanolamine	190–192
MDEA-CO ₂ -water system, CO ₂ partial	cylindrical pores, 187–190
pressures for, 139–140	$N_{layer}vs. R_{ex}/L_0$ in, phase separation of
MD simulation, atomistic, 87, 89	diblock copolymer, 201–204, 209
Meso-scale, 4	and SSL theory, conflict between, 206
Mesoscale clusters and dispersed particles,	MRE. See Modified Reynolds equation
exchange between, 8	Multiphase chemical reactor, 2–4
Meso-scale/continuum-level modeling	Multiphase flow in fluidized bed reactors
tool, 81–83	10–11
Meso-scale modeling, macro-scale	Multiphenomena in gas diffusion layer,
influence into, 15	97–102
Meso-scale structures, 2	"Multi-scale CFD"
classic chemical engineering models for,	applications
10	periodic domain simulations,
of copolymer materials, 155	16–21
critical effect of, 8–9	scope of, 23–24
drag coefficient and mass transfer for	simulations of risers and validations,
CFB due to, 8–9	21–23
in gas–solid suspensions, 13	correlative
particle behaviour in, 4	challenges associated with, 14–15
related to processes, 155	computation cost effectiveness of, 13
spatiotemporal features of	paradigms for, 12
dynamic characterizations, 6–8	for single-phase turbulent flows, 12
time-averaged characterization, 5–6	subparticle simulations using,
TFM grid refining and, 23–24	12–13
two-phase description of, 5–6	definition, 12
<i>n</i> -Methyldiethanolamine, 145	variational
CO ₂ capture with, 137–138	challenges to, 15–16
molecular structure of, 137	definition of, 15
Microkinetics-based reactor models, 135	scale separation condition in, 15
Micro-phase structure formation	Multi-scale modeling
mechanism for block copolymers, 184	approaches, candidates for evaluating
Micro-scale, 4	HDD system, 66–74
MIP reactor, industrial	PEFC, 63–66
flow regime diagram of, 46	at atomistic/molecular level, 76–81
simulation of, 45	bridging methodology, 85–87
solids volume fraction in laboratory-	of chemical supply chain, 122
scale cold model of, 44	components, 74–75
Mixing process of chain-like molecular	demand for research in, 113
systems, 160	at meso-scale/continuum level, 81–83
Modified Reynolds equation, 109	as multidisciplinary analysis paradigm
Molecular dynamics, 78	60
and MC, 78	at process-scale level, 83–84
molecular motion in, 79–81	publications on, 62
Molecular system, 75	at quantum level, 75–76
Molecular thermodynamic model, 156	schematic description of, 61
	the second of th

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	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
publications on, 62	two-phase flow, 18
time and length scales in, 62	PFPE lubricant films, coarse-grained,
Multi-scale simulation, 61	bead-spring model of, 104–105
Multi-scale structures, 2	PFPE molecule
N.C. B.C.	oligomeric, rigid units of, 89–90 PFPE Zdol molecule, molecular model
Nafion®, 65	of, 105
Nanoanalysis, advances in, 60	radius of gyration of, 108
Nanopore	PFPEs, functional and nonfunctional
Helmholtz energy confined in, 187	endbead density profiles for, 106–107
layer transitions in, 204	spreading profile of SRS models with,
Negative pressure heads, 73	107
Nonlinear nonequilibrium system, 16	PFPE systems, 71
	and disk overcoat, interaction between, 71–72
Objective functions, 127	bonding mechanism between, 72
Ono–Kondo equation, 177	DDPA-S, DDPA-D, and ZTMD, 72
Optimization methods, 127–128	molecular conformation of, 108
	Physical system, multi-scale/holistic
	interpretation of, 101
Parameter cases, 128–129	Piperazine, 137
Particle–particle interaction, 11	Plug-flow model, 10
PEFC. See Polymer electrolyte fuel cells	PNIPAm gels, swelling ratio of, 175
PEFC-based power plant, process-level	Polymer adsorption
model of, 64	based on lattice or off-lattice model, 176
PEFC model	at interface, importance of, 176
device-level, 102	lattice-based theories for, 177
multiphenomena in gas diffusion layer,	DFT, 177
97–102	general formalism for, 178–179
polymer electrolyte membrane	LDFT, 177–182
ab initio models of, 93	at solid–liquid interface, 182–184
composition of, 92–93	Polymer chains, residual Helmholtz
water uptake variation in, 94–96	energy of dissociation and association
process-level, 102–103	of, 166–167
water management strategies in, 65–66	Polymer electrolyte fuel cells
PEM. See Polymer electrolyte membrane PEM materials	component of, 63
functions, 65	design, 66
Nafion [®] , 65	key issues in making paradigm shift in, 66
PEM systems, water management issues	Polymer electrolyte membrane, 63
in, 66	ab initio models of, 93
Periodic domain simulations, periodic 2D	components of, 92
domains, 16	composition of, 92–93
domain-size dependency of, 20	water uptake variation in, 94–96
grid-size dependency of, 20–21	Polymer systems
o	,

based on lattice fluid model, equation of Helmholtz energy of symmetrical parallel lamellar confined in, 193-196 state for, 171-173 close-packed lattice model for, 159 ROMs. See Reduced-order models comparisons with molecular simulation results coexistence curves, 168-170 Sector column structure Helmholtz energy of, 198-199 critical temperature and critical volume fraction, 167-168 Semilean and lean solution columns, 147 liquid-liquid phase equilibria, Sequential modular (SM) modeling and 170-171 equation-oriented (EO) modeling, 123 Helmholtz energy of, 178 "Simulate" cases, 128 Helmholtz energy of mixing of, 167 Slip velocity Polystyrene-b-polybutadiene (PS-b-PBD) asymptotic, 19 grid resolution effects on, 18-19 diblock copolymers confined in nanopore periodic domain size effects on, 19 comparison with MC simulation and Solid particles, heterogeneity in, 6 SSL theory, 201-204 SRS models, 89-90, 91 Helmholtz energy profiles of, 200-201 with spins, 108 morphologies of, 199 spreading profile of PFPEs, 107-108 Primary reformer feed steam to carbon SSL theory. See Strong Segregation Limit (S/C) ratio, 147 theory Process economics, 132 Static structures, microscale difference of, 5 Process-scale models, 83-84 Strong Segregation Limit theory, 185 for diblock copolymers confined in PS/cyclohexane systems, spinodal curves ring-like curved surfaces, 193-199 and coexistence curves of, 174 PZ. See Piperazine Helmholtz energies predicted by, 205-206 $N_{laver}vs. R_{ex}/L_0 in, 201-204$ Quantum level models phase separation of confined diblock coupling of, 87-89 copolymer, 209-210 quantum level models, 75-76 Subgrid structure modeling, 23 Subparticle simulations, 12–13 Symmetrical concentric-ring barrel Real-time optimization (RTO) applications, structure Helmholtz energy of, 193-196 134 Symmetrical concentric square column Reconcile case, 129 Reconciliation models, 126-127 structure, Helmholtz energy of, Reduced-order models 207 - 208approximation errors, 87 different forms of, 86-87 linking models at various scales using, Ternary Ising lattice internal energy of mixing for, 166 Ternary polymer solutions, liquid-liquid role of, 86 Representative elementary volume (REV) equilibria phase diagrams of, 170-171 TFM. See Two-fluid model method, 97, 98 Reverse Monte Carlo (RMC) techniques, 88 Thermal 40 mers, total segment-density Ring-like curved surfaces, 192 distributions of, 184 Helmholtz energy of asymmetrical parallel Tribology, 66-67 lamellar confined in, 196-198 Turbulent flows, transfer of energy in, 15 Helmholtz energy of sector column Two-fluid model. See also Periodic domain confined in, 198-199 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

Vapor–liquid equilibria for propanol + [Me₃BuN][NTf₂] system, 175 Variational multi-scale CFD challenges to, 15–16 and correlative, comparison between, 17 definition of, 15 scale separation condition in, 15

Water uptake variation in PEM, 94-96

Ztetraol multidentate, 72 ZTMD. See Ztetraol multidentate