

Contents

Preface	<i>page xiii</i>
Notation	xvii
1 Introduction	1
1.1 Disperse multiphase flows	1
1.2 Two example systems	3
1.2.1 The population-balance equation for fine particles	3
1.2.2 The kinetic equation for gas–particle flow	8
1.3 The mesoscale modeling approach	14
1.3.1 Relation to microscale models	16
1.3.2 Number-density functions	18
1.3.3 The kinetic equation for the disperse phase	19
1.3.4 Closure at the mesoscale level	20
1.3.5 Relation to macroscale models	20
1.4 Closure methods for moment-transport equations	23
1.4.1 Hydrodynamic models	23
1.4.2 Moment methods	25
1.5 A road map to Chapters 2–8	27
2 Mesoscale description of polydisperse systems	30
2.1 Number-density functions (NDF)	30
2.1.1 Length-based NDF	32
2.1.2 Volume-based NDF	33
2.1.3 Mass-based NDF	33
2.1.4 Velocity-based NDF	34
2.2 The NDF transport equation	35
2.2.1 The population-balance equation (PBE)	35
2.2.2 The generalized population-balance equation (GPBE)	37
2.2.3 The closure problem	37
2.3 Moment-transport equations	38
2.3.1 Moment-transport equations for a PBE	38
2.3.2 Moment-transport equations for a GPBE	40
2.4 Flow regimes for the PBE	43
2.4.1 Laminar PBE	43
2.4.2 Turbulent PBE	44
2.5 The moment-closure problem	45

3	Quadrature-based moment methods	47
3.1	Univariate distributions	47
3.1.1	Gaussian quadrature	49
3.1.2	The product–difference (PD) algorithm	51
3.1.3	The Wheeler algorithm	53
3.1.4	Consistency of a moment set	55
3.2	Multivariate distributions	62
3.2.1	Brute-force QMOM	63
3.2.2	Tensor-product QMOM	68
3.2.3	Conditional QMOM	74
3.3	The extended quadrature method of moments (EQMOM)	82
3.3.1	Relationship to orthogonal polynomials	83
3.3.2	Univariate EQMOM	84
3.3.3	Evaluation of integrals with the EQMOM	91
3.3.4	Multivariate EQMOM	93
3.4	The direct quadrature method of moments (DQMOM)	99
4	The generalized population-balance equation	102
4.1	Particle-based definition of the NDF	102
4.1.1	Definition of the NDF for granular systems	102
4.1.2	NDF estimation methods	105
4.1.3	Definition of the NDF for fluid–particle systems	107
4.2	From the multi-particle–fluid joint PDF to the GPBE	110
4.2.1	The transport equation for the multi-particle joint PDF	111
4.2.2	The transport equation for the single-particle joint PDF	112
4.2.3	The transport equation for the NDF	112
4.2.4	The closure problem	113
4.3	Moment-transport equations	114
4.3.1	A few words about phase-space integration	114
4.3.2	Disperse-phase number transport	116
4.3.3	Disperse-phase volume transport	116
4.3.4	Fluid-phase volume transport	117
4.3.5	Disperse-phase mass transport	118
4.3.6	Fluid-phase mass transport	121
4.3.7	Disperse-phase momentum transport	123
4.3.8	Fluid-phase momentum transport	124
4.3.9	Higher-order moment transport	127
4.4	Moment closures for the GPBE	130
5	Mesoscale models for physical and chemical processes	136
5.1	An overview of mesoscale modeling	136
5.1.1	Mesoscale models in the GPBE	137
5.1.2	Formulation of mesoscale models	141
5.1.3	Relation to macroscale models	145
5.2	Phase-space advection: mass and heat transfer	147
5.2.1	Mesoscale variables for particle size	149
5.2.2	Size change for crystalline and amorphous particles	152
5.2.3	Non-isothermal systems	155
5.2.4	Mass transfer to gas bubbles	156

5.2.5	Heat/mass transfer to liquid droplets	158
5.2.6	Momentum change due to mass transfer	160
5.3	Phase-space advection: momentum transfer	161
5.3.1	Buoyancy and drag forces	162
5.3.2	Virtual-mass and lift forces	171
5.3.3	Boussinesq–Basset, Brownian, and thermophoretic forces	173
5.3.4	Final expressions for the mesoscale acceleration models	175
5.4	Real-space advection	177
5.4.1	The pseudo-homogeneous or dusty-gas model	179
5.4.2	The equilibrium or algebraic Eulerian model	180
5.4.3	The Eulerian two-fluid model	181
5.4.4	Guidelines for real-space advection	182
5.5	Diffusion processes	183
5.5.1	Phase-space diffusion	184
5.5.2	Physical-space diffusion	187
5.5.3	Mixed phase- and physical-space diffusion	188
5.6	Zeroth-order point processes	189
5.6.1	Formation of the disperse phase	189
5.6.2	Nucleation of crystals from solution	191
5.6.3	Nucleation of vapor bubbles in a boiling liquid	191
5.7	First-order point processes	192
5.7.1	Particle filtration and deposition	193
5.7.2	Particle breakage	195
5.8	Second-order point processes	202
5.8.1	Derivation of the source term	203
5.8.2	Source terms for aggregation and coalescence	205
5.8.3	Aggregation kernels for fine particles	206
5.8.4	Coalescence kernels for droplets and bubbles	212
6	Hard-sphere collision models	214
6.1	Monodisperse hard-sphere collisions	215
6.1.1	The Boltzmann collision model	217
6.1.2	The collision term for arbitrary moments	218
6.1.3	Collision angles and the transformation matrix	221
6.1.4	Integrals over collision angles	223
6.1.5	The collision term for integer moments	230
6.2	Polydisperse hard-sphere collisions	236
6.2.1	Collision terms for arbitrary moments	237
6.2.2	The third integral over collision angles	242
6.2.3	Collision terms for integer moments	243
6.3	Kinetic models	246
6.3.1	Monodisperse particles	246
6.3.2	Polydisperse particles	248
6.4	Moment-transport equations	250
6.4.1	Monodisperse particles	251
6.4.2	Polydisperse particles	255
6.5	Application of quadrature to collision terms	261
6.5.1	Flux terms	261
6.5.2	Source terms	263

7	Solution methods for homogeneous systems	266
7.1	Overview of methods	266
7.2	Class and sectional methods	269
7.2.1	Univariate PBE	269
7.2.2	Bivariate and multivariate PBE	279
7.2.3	Collisional KE	283
7.3	The method of moments	289
7.3.1	Univariate PBE	290
7.3.2	Bivariate and multivariate PBE	296
7.3.3	Collisional KE	297
7.4	Quadrature-based moment methods	300
7.4.1	Univariate PBE	301
7.4.2	Bivariate and multivariate PBE	307
7.4.3	Collisional KE	314
7.5	Monte Carlo methods	315
7.6	Example homogeneous PBE	319
7.6.1	A few words on the spatially homogeneous PBE	319
7.6.2	Comparison between the QMOM and the DQMOM	323
7.6.3	Comparison between the CQMOM and Monte Carlo	324
8	Moment methods for inhomogeneous systems	329
8.1	Overview of spatial modeling issues	329
8.1.1	Realizability	330
8.1.2	Particle trajectory crossing	332
8.1.3	Coupling between active and passive internal coordinates	335
8.1.4	The QMOM versus the DQMOM	337
8.2	Kinetics-based finite-volume methods	340
8.2.1	Application to PBE	341
8.2.2	Application to KE	345
8.2.3	Application to GPBE	347
8.3	Inhomogeneous PBE	349
8.3.1	Moment-transport equations	349
8.3.2	Standard finite-volume schemes for moments	350
8.3.3	Realizable finite-volume schemes for moments	353
8.3.4	Example results for an inhomogeneous PBE	358
8.4	Inhomogeneous KE	362
8.4.1	The moment-transport equation	363
8.4.2	Operator splitting for moment equations	363
8.4.3	A realizable finite-volume scheme for bivariate velocity moments	364
8.4.4	Example results for an inhomogeneous KE	366
8.5	Inhomogeneous GPBE	373
8.5.1	Classes of GPBE	373
8.5.2	Spatial transport with known scalar-dependent velocity	376
8.5.3	Example results with known scalar-dependent velocity	377
8.5.4	Spatial transport with scalar-conditioned velocity	381
8.5.5	Example results with scalar-conditioned velocity	388
8.5.6	Spatial transport of the velocity-scalar NDF	396
8.6	Concluding remarks	401

Appendix A Moment-inversion algorithms	403
A.1 Univariate quadrature	403
A.1.1 The PD algorithm	403
A.1.2 The adaptive Wheeler algorithm	404
A.2 Moment-correction algorithms	405
A.2.1 The correction algorithm of McGraw	405
A.2.2 The correction algorithm of Wright	407
A.3 Multivariate quadrature	408
A.3.1 Brute-force QMOM	408
A.3.2 Tensor-product QMOM	410
A.3.3 The CQMOM	412
A.4 The EQMOM	413
A.4.1 Beta EQMOM	413
A.4.2 Gamma EQMOM	416
A.4.3 Gaussian EQMOM	418
Appendix B Kinetics-based finite-volume methods	421
B.1 Spatial dependence of GPBE	421
B.2 Realizable FVM	423
B.3 Advection	427
B.4 Free transport	429
B.5 Mixed advection	434
B.6 Diffusion	437
Appendix C Moment methods with hyperbolic equations	441
C.1 A model kinetic equation	441
C.2 Analytical solution for segregated initial conditions	442
C.2.1 Segregating solution	442
C.2.2 Mixing solution	443
C.3 Moments and the quadrature approximation	444
C.3.1 Moments of segregating solution	444
C.3.2 Moments of mixing solution	446
C.4 Application of QBMM	447
C.4.1 The moment-transport equation	447
C.4.2 Transport equations for weights and abscissas	448
Appendix D The direct quadrature method of moments fully conservative	450
D.1 Inhomogeneous PBE	450
D.2 Standard DQMOM	450
D.3 DQMOM-FC	453
D.4 Time integration	455
References	459
Index	488